

Atom – Bond Organization Theory and a New Intermolecular Force for Applications Such as Ultrahydrophobic Materials

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Abstract

A new intermolecular force comparable to Van Der Waals force leads to high friction in amorphous nanopowders of silica. The radial distribution function can be applied both at particle-to-particle level as well as atoms/molecules inside a nanoparticle usually amorphous nanoparticle. Hydrophobic performance and corrosion control can be of big impact with high intermolecular force intensity. Here we also study friction due to this force in terms of powder rather than bulk materials friction property. High friction, high Van Der Waals related intermolecular force and unusual high repulsion between nanoparticles clinches the existence of this force. The ultrahydrophobic performance with near maximum water contact angle positions this field for corrosion control in vast application contexts. We conclude with a discovery of a new intermolecular force only in amorphous nanopowders and its relevance as a nanotechnology application research also.

Keywords: Nanopowder, silica, Intermolecular force, Ultrahydrophobic, Lennard-Jones potential. Radial Distribution Function (RDF).

INTRODUCTION

Superhydrophobic surfaces are suited for theoretical and application contexts. To some extent high Intermolecular Forces and surface morphology have a role in hydrophobic property. They can be used in aeronautical, land transport and seagoing vessels [1] and also in pipelines, also in water and ambient civil structures. In hydrophobic materials with surface roughness in material, the water contact zone has air cavities between water drop/liquid and physical surfaces above transport materials, therefore without enough water contact area, corrosion is lower. The atom – bond organization theory and its high intermolecular force make it relevant for massive decrease in corrosion. Superhydrophobic surfaces and study of corrosion electrochemistry is an active area of research. However very high intermolecular forces in materials such as amorphous silica - SiO₂ nanoparticles is an extraordinary window of opportunity for Superhydrophobic surfaces and further to decrement corrosion activity in a big way. The most interesting part of this is that we can have superhydrophobic surfaces with mechanical stability of surface structure along with tailored morphology [2]. So we

get to keep the water environment but little corrosion takes place. Also, superhydrophobic material reduces the surface area of wetting and have a –via “air film” which decreases corrosion with high potential in applications.

We can get Ultrahydrophobic performance from this high intensity intermolecular force. Water based applications can have minimized corrosion due to hydrophobic property on surface of structures/materials. Corrosion is 3.4% of global GDP and it is 4.2% of India's GDP. With such high economic value based on hydrophobic performance, the new intermolecular force is ripe area for further studies and vast applications [3]. We hence developed the theory for this intermolecular force.

LITERATURE SURVEY

FRICITION

Previous studies [4] have shown high friction in silica nanopowders during PM - Powder Material compaction. The study of ferrous based Distalloy powders showed that [5] as the density of PM Compact increases the friction decreases. The stress of die walls is half of axial stress applied by punch on PM compact - or nearly so. At pressures above 200 MPa large experimental variations in friction on die wall means better dies and better accuracy to measure friction. While friction is stable at high pressure, the experimental variation at high pressure due to design and measurement method. The study and analysis by Turenne, S. et. al. [6] showed that at later stages of compaction, the ratio of axial and radial stress, z is constant. They calculated the friction and stress with an analytic model which relates to powder compaction only and not bulk material parameter(s) viz. if powder size, shape etc changes the friction force changes for even for same material composition. This approach of friction and stresses for nanopowder compaction of silica, SiO₂ nanopowders has been carried out. The friction depends only on van der Waals force and shape, morphology, roughness. Here only spherical nanopowders only, so only VDW is valid. So change in Intermolecular force only decides friction at 12nm, 20nm and 53 μ m[7]. The study by [7] showed that friction is more in thin SiO₂ film or Si than thick SiO₂. When compared to Si wafer, thin SiO₂ film on Si wafer led to more friction than even thick SiO₂ film even though the roughness was same for both. The

studies used AFM with blunted tip, clear proof that friction is influenced by Van Der Waals (though surface roughness always has a role in friction). The AFM tip is made of Silicon Nitride, Si_3N_4 , hence it has hydrophobic surface chemistry similar to SiO_2 leading to more friction. Hydrophobic tip has more friction with AFM tip made of Si_3N_4 , so it has more hydrophobic nature. The work of Johnson [9] gives contact mechanics relations for forces at contact point between surfaces. High forces lead to high friction as contact points experience the force through friction. It shows field of force at contact point can be calculated, just like surface contact mechanics, the volume forces of Van Der Waals would also lead to friction at contacts such as the forces we see in PM compaction of nanopowder. An advanced study with sophisticated equipment by Tien, Yong-Ming et al. [10] used bentonite in compaction and it was ejected while forces and friction were measured in entire process using load cell in the equipment. The friction ratio was more or less constant for bentonite of different origin. Special measurement equipment led to results consistent with previous research studies and Analytical models. Existing analytical models fully valid including the one applied to this silica nanopowder study. Fig. 1 shows silica nanopowders in SEM study.

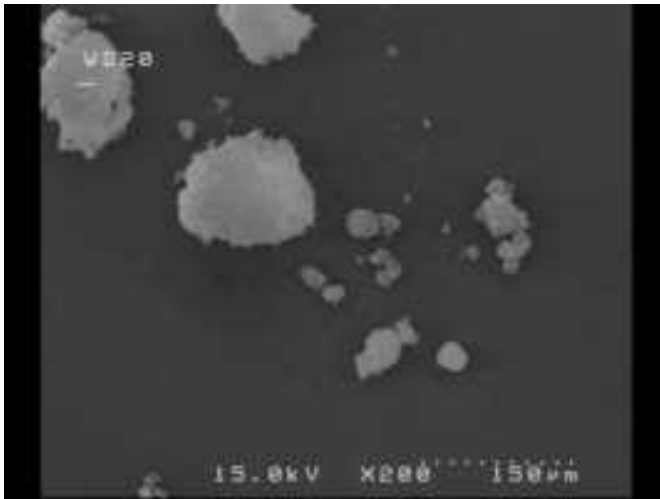


Fig. 1: SEM image of Aerosil 200 silica nanopowder

VAN DER WAALS

The Van Der Waals potentials for various materials and combinations therein including silica with silica itself, VDW interaction and constants for the VDW potential are provided in Sarapat, Pakhpoom, Ngamta Thamwattana & Duangkamon Baowan [11]. The van der Waals force of silica showed that silica can adhere with paint – usage in construction industry. The VDW of silica and as a measure of its hydrophobic property in applications. Hence we can have corrosion control with hydrophobic aspect of nano silica is apparent. In the study of [12] the nanoparticle potential with Lennard – Jones 6 – 12 relation is modified with one more term. The joint between two nanoparticles is not actually 2 full spheres but a – “Janus dumbbell” shape. Physical property is an anomaly in Lennard – Jones for nano but with

correction term, the diffusion value anomaly is less. The new atom – bond organization theory is relevant for non-spherical 2 atoms combination, the changes to L- J, 6 – 12 and diffusion imply a new and different theory and/or phenomenon for nanopowder of silicon. In the Van Der Waals potentials [13] between two silica nanoparticles – there is a deeper potential well and larger separation for large – size 20 nm nanoparticle. The interaction is lower in energy and has smaller separation in particle – to – particle potential of nano silica SiO_2 particles. However that computer model does not specifically assume amorphous nature of silica nanoparticles. Generally nanoparticle aggregates of loose and irregular form in research computer model of Thirunavukkarasu Asaimuthu [4]. However in the article of [13], it shows magic number of particles in –pseudo “atoms” as spherical aggregates only.

There is high Van Der Waals intensity in data of 20nm silica [14]. The MD simulation and experimental study verified the agreement of VDW forces in silica by both methods. This data is close to Thirunavukkarasu Asaimuthu [4] data of nano silica though latter has a nanosize of 12nm. Further comparison with macro silica powder shows orders of magnitude of many decades difference between nano silica and bulk silica. In [15], the pair potential for nanoparticles in polymer ligand (composed of nanoparticle composite in polymer ligand) and SEM was used to get pair potential from the Radial Distribution Function [RDF]. Even though there are different sizes of nanoparticles there is a large overlap in pair potential since matrix ligand decided pair potential. So even in different areal densities of nanoparticles, the radial distribution function (RDFs) is same. This study shows that in mixtures, either nanoparticles alone or ionic graft only i.e. polymer only can fix pair potential derived from the RDF. The Molecular Dynamics simulation [16] of forces between silica, SiO_2 nanoparticles in an electrolytic medium was carried out with varying amounts of background ions. This research shows that water can penetrate the silica nanoparticles and formation of agglomerates will suit fractal analysis. The thesis of Thirunavukkarasu. A. [4] research showed that the formation of aggregates in loose form in air which was apparent in the powder can of silica nanopowder, even at Macro level, it has the ability to fill can again through some of the nanopowder was taken out of the can. The fact that amorphous nanosilica is influenced by ions in electrolyte means that Van Der Waals forces at work while magnitude is not shown. Silica is non-ionic hence only VDW can interact with ions in electrolyte.

RADIAL DISTRIBUTION FUNCTION

The computer model [17] of amorphous silica and crystalline silica i.e. cristoballite showed changes in RDFs and bond angles. At smaller nanosizes the surface effects and surface “-OH” groups effects are more “-OH” surface groups are more in number. Thus the surface effect in nano silica is seen in the change in RDFs and bond angles change, however there was no change in density including experimentally measured density, hence at same density of SiO_2 , RDFs and bond angles can change – that is so in principle. The study [18] with synchrotron based X-Rays and X-Ray data was used to

obtain Atomic RDF. Synchrotron X-Rays can measure XRD – X-RAY Diffraction at lower frequency than $Cu_{K\alpha}$ as well as $Ag_{K\alpha}$, hence we get more useful and powerful data and leads to analysis studies silica RDF has low error and low residual information in data from Synchrotron XRD. So Silica, SiO_2 well suited for RDF analysis. The research on Phases in [19] shows pair distribution function $g(r)$ and difference pair distribution function corresponding to Fe – O in FeO_6 shows that matrix and nanocomposite of FeOOH in amorphous silica Matrix are different in structure FeO_6 is formed in nanocomposite which is seen in difference pair distribution function, $\Delta g(r)$. The matrix rigidity restricts growth of FeOOH at 4 nm size maximum. The power of synchrotron XRD and use of pair distribution function for structure – phases from SAXS is proved. Along similar lines the RDF can be applied at particle – to – particle level also.

HYDROPHOBIC PERFORMANCE

The hydrophobic property was the focus of the study by Emami, Fateme.S., et. al., [20]. Silica was simulated for various properties with Gibbs ensemble. Water contact angle in model was fully accurate along with data from other sources – hydrophobic nature of silica is exhibited in this model. Difficulties were seen with van Der Waals parameters mentioned in this research.(this has aerosil silica study here in this research), so we need the phenomenon of new intermolecular force to make this accurate scientifically and systematically. The hydrophobic property to reduce corrosion [3] was reviewed with other sources research in this article. The stable and self-heal & inhibitor loaded hydrophobic surfaces is considered for corrosion protection. This new intermolecular force would be a vital approach for such advanced protection. A vast array of materials and processes are addressed, but this intermolecular force will be a materials science solution for hydrophobic coating while these processes and materials are biomimetic and spell out the needs for their research field. The review of the Hydrophobic research and the requirements of an advanced Hydrophobic material were spelt out in the article by Thirunavukkarasu. A., and Pankaj. B. Tambe [20]

FRICITION in nano and microscopic silica, SiO_2

The friction in nanopowder of silica is high. This friction is not that of bulk monolithic silica or even the single particle material of nanosilica but more connected to a green compact of silica but atomic bonding is only inside each nanoparticle but particles in powder and its green compact do not have particle to particle bond on an atom to atom way but instead have intermolecular forces across particles but maybe longer range than interatomic bonding of atoms inside each nanoparticle. My research [22] on AFM of silica nanopowder compaction in the past showed that local elastic moduli measurement on AFM was smaller than that of bulk silica. This work also showed that with increasing compaction force, the green density of compact increases and the value of break point of green compact also increases as force of compaction increases. The friction here is particulate powder during

compaction in a die resulting from intermolecular forces and not even the shape and morphology of silica nanoparticle. Bulk silica has friction with a combination of van der waals of silica as well as shape and morphology, surface roughness of monolith of silica. However this friction is determined by intermolecular forces in nanosize silica, SiO_2 powder and the powder has spherical nanoparticles only.

We calculate the friction with the analytical relation [6] provided by Turenne et.al..

$$p(x) = p(0)\eta^{\frac{x_i}{d}} \quad (1)$$

x_i = Distance from upper punch.

$P(0)$ = applied pressure at upper punch surface, and also d = part diameter

η is slide coefficient relation of the applied pressure to transmitted pressure

$$\eta = \exp(-4\mu z) \quad (2)$$

Z is a constant at points close to maximum pressure at end of compaction, and also μ = coefficient of friction

The force equations are

$$E = \left(\frac{Stress}{Strain} \right) \quad (3)$$

$$\epsilon_x = ((1/E)(\sigma_x - 2\nu\sigma_r)) \quad (4)$$

$$\epsilon_r = (1/E)((1-\nu)(\sigma_r - \nu\sigma_x)) \quad (5)$$

$$\nu = 0.05 \rho - 0.107 \quad (6)$$

Strain

$$\epsilon_x = ((1/E)(\sigma_x - 2\nu\sigma_r)) \quad (4)$$

$$\epsilon_r = (1/E)((1-\nu)(\sigma_r - \nu\sigma_x)) \quad (5)$$

$$\nu = 0.05 \rho - 0.107 \quad (6)$$

$$Z = \left(\frac{\sigma_r}{\sigma_x} \right) = \left(\frac{\nu\epsilon_x + \epsilon_r}{(1-\nu)\epsilon_x + 2\epsilon_r} \right) \quad (7)$$

$P(0)$ is 140 MPa at point 1 at the end of densification, & $p(0)$ is 130MPa at the penultimate point of densification. We consider two values of x , and x at 1mm and $x=2$ mm to calculate η . We get ratio of μ_1 & μ_2 at these two x values. Then we consider $x=0$ and do (1) again to get η_1 η_2 . then we get $\mu_1 = 2 \mu_2$

Then we get ν from (6) with relative density.

We get ϵ_x & ϵ_r from (4) & (5). We use (7) to obtain $-z$. Further we get μ_1 & μ_2 from (2)

The data and results:

Table 1: Friction in nanosize and micronsize powders

Friction	d = 12nm	d =53 μm
μ_1	0.00656	0.00023
μ_2	0.00328	0.00011

These are the friction data of flowing powder/nanopowder material, not bulk monolithic material.

So the friction in an nanopowder is about 30 to 35 times higher than the microscopic/micron size powders of silica i.e. friction is more than an order of magnitude in nanopowder of amorphous silica when compared to micron size silica powder.

The research of Lessel, Matthias, et. al.,[8] clearly shows friction is highly because of van der Waals intermolecular forces and this order of magnitude difference between macroscopic silica

SiO₂ and nanopowders of silica, SiO₂ is a clear evidence of a new intermolecular force with amorphous nanoparticles.

The interaction energy per unit area is given by:

$$\phi_{vdw}(x) = (-A_i/M_{ij}) / (12\pi x^2)$$

With the Hamaker constant A_i/M_{ij} .

The use of Hamaker constant in L – J, 6 – 12 potential in my research previously [4] and this research article rightly specifies the need to determine not theoretically but additional terms in their thin film of nanosize and also Lennard – Jones Interatomic potential and use of water contact angle (Hydrophobicity) all are mounting evidence of this new intermolecular force in amorphous silica nanopowder.

They clearly state that ultrathin nanofilms of SiO₂ on silicon wafer need to change the Hamaker constants such as by using water contact angle proves that it is likely a new advanced high value magnitude Intermolecular Force i.e. When there is a large change in amount of force, it is a change in kind of force and not just the same force with higher quantity – viz – a new intermolecular force.

While Hamaker [4] specified a maximum of (4×10^{-23} j nm⁻⁶) and minimum of (1×10^{-25} J nm⁶) in his article, we used the attractive term constant of 12×10^{-24} J nm⁶ in the Lennard – Jones 6 – 12 potential which is very close to maximum value as per Hamaker to produce successful model of Agglomerate formation in nanopowder of amorphous silica. We conclude that my thesis and above article of Matthias Lessel et. al., and its prescription to constants in L-J,

6 – 12 potential establish the sound basis of this new intermolecular force. The energy values in this AFM study compare to be smaller than my thesis [4] and hence being nanoparticles rather than thin films in Matthias Lessel., et. al., explain the veracity of the Atom – Bond organization theory and the discovery of this new intermolecular force. All friction values are for nanopowder material in die compaction and not for bulk silica glass or nanostructured film of nanothick silica - thin film material. It is in terms of powder compacted in die and not a rigid monolithic material value.

Both microsize and nanosize SiO₂ are spherical, so only Van Der Waals affects wall friction and surface roughness of micron size Silica [SiO₂] is not an issue, also dies are made of steel for both nano and microsize compaction. So we can safely surmise that the friction measured here is only due to material nature of respective powders viz. VDW and surface forces of nanosize and microsize silica, SiO₂ as friction on surface only in relative terms if not absolute terms.

All metals have much higher – usually multiples of silica, SiO₂ VDW, the variation in die walls in microsize and nano silica compaction is small role, the considerable variation of friction of the scale of one order of magnitude is due silica particle size as 53 μ and 12nm only. Hence the variation of friction in PM compaction is due to nanosize silica material property. The steel dies are same class of materials and VDW values for dies used in compaction are close to each other. And the order of magnitude higher friction in nanosilica is an indication of friction from nanosilica with much higher and a new type of intermolecular force in nanosilica and it is manifested in this friction data.

Thus the atom – bond organization theory and a new Intermolecular Force are glaringly evident in Friction data both by PM compaction and reports of AFM friction in its probe by Matthias Lessel et. al. [8]

High Van Der Waals Forces

The Van Der Waals forces of nanosize silica, SiO₂ and micron size silica powder are compared to analyse InterMolecular forces. The VDW potential is described with the quantitative terms of Lennard– Jones potential with two terms. The first term has radius with an exponent of 12 and is positive for repulsive force. The second term is radius with an exponent of 6 and is negative signifying the attractive term. Both terms have the radius in the denominator and the constant for each term is in the numerator of r^{-12} and r^{-6} terms i.e. the repulsive and attractive terms respectively. This is known as the Lennard – Jones, 6 – 12 potential used for Van Der Waals forces.

The thesis of Thirunavukkarasu Asaimuthu [4] provides the L-J potential for 12nm silica. The Ph.D Thesis of [14] provides the L- J potential of 20nm nanosize silica powder. The [11] provides microsize material –ve term, L – J potential i.e. micron silica.

The data:

Table 2: Van Der Waals potential, its constants in different nano and one micronsized silica, SiO₂

Particle diameter	+ve term L-J Potential constant of r ¹² In J/molecule nm ¹²	-ve term L-J potential constant of r ⁶ J/molecule nm ⁶
d = 12 nm	32 x 10 ⁻²⁷	12 x 10 ⁻²⁴
d=20 nm	6.147 x 10 ⁻²⁶	8.492 x 10 ⁻²⁴
d = μm microsize	5.143 x 10 ⁻²	2.617 x 10

The microscopic (d=53 μm) value terms are for solid silica surface in paint, so it is microscopic silica and not nano silica.

There is a 25 orders of magnitude difference between nanosilica as well as microsilica. This is same for both repulsive r¹² and also attractive r⁶ terms. Both terms have the same 25 orders of magnitude difference in each of repulsive and attractive terms of L - J 6 - 12 potential.

The data for micron size is for microsize material which is like a micron or higher thickness coating such as paint etc. it is indicative of values of L - J, 6 - 12 constants for micron - size silica, SiO₂ materials. This is valid as above a size of 1 μm, the interatomic potentials are same as bulk materials of silica & for practically all materials being - "bulk". The interatomic and atomic potentials only become variable only, at 100nm nano or similar near nano size of the material. At 1μm size and above, the material and its atomic/interatomic potentials are constant in those sizes i.e. in microsize materials. So the VDW data of microsize silica for microscopic structure of silica - to - silica interactions is valid for micron size powder and other microsize material of silica.

Next an estimation of interatomic potential of Intermolecular forces is now done for powder size r = 1nm.

For Thirunavukkarasu Asaimuthu [4] the VDW is -11,968 x 10⁻²⁷ J/molecule nm²

In the case of Ph.D research of Meng[14] the Van Der Waals at 1nm particle is - 606.19 x 10⁻²⁴

J/molecule nm²

While for micronsized silica at r = 1nm the VDW is 4.3 x 10⁻⁴⁶ J/molecule nm²

The highest value of VDW potential is seen in MD Simulation of 20nm particle size [14]

Followed closely by 12nm particle size nanosilica in [4] MS Thesis.. The bulk micronsized silica has very low VDW forces in comparative terms. The nano silica has 68 orders of magnitude higher VDW per molecule. So a new entirely different phenomenon is seen in nanosize silica, hence we

conclude that there exists a new intermolecular force and atom - bond organization theory in nanosize silica particles. With only about 2 orders of magnitude variation in VDW between [4] and [14], we conclude the new intermolecular force is proved in nanometer range amorphous SiO₂ powder size. But at bulk silica, the change is i.e. decrease in VDW is 22 orders of magnitude and hence conventional VDW is only force in bulk silica. The atom bond organization and new intermolecular force both stand proved. The Relation for particle - to - particle Van Der Waals from molecule-to-molecule Van Der Waals and its analytical process is shown in Fig. 2 and Fig.3.

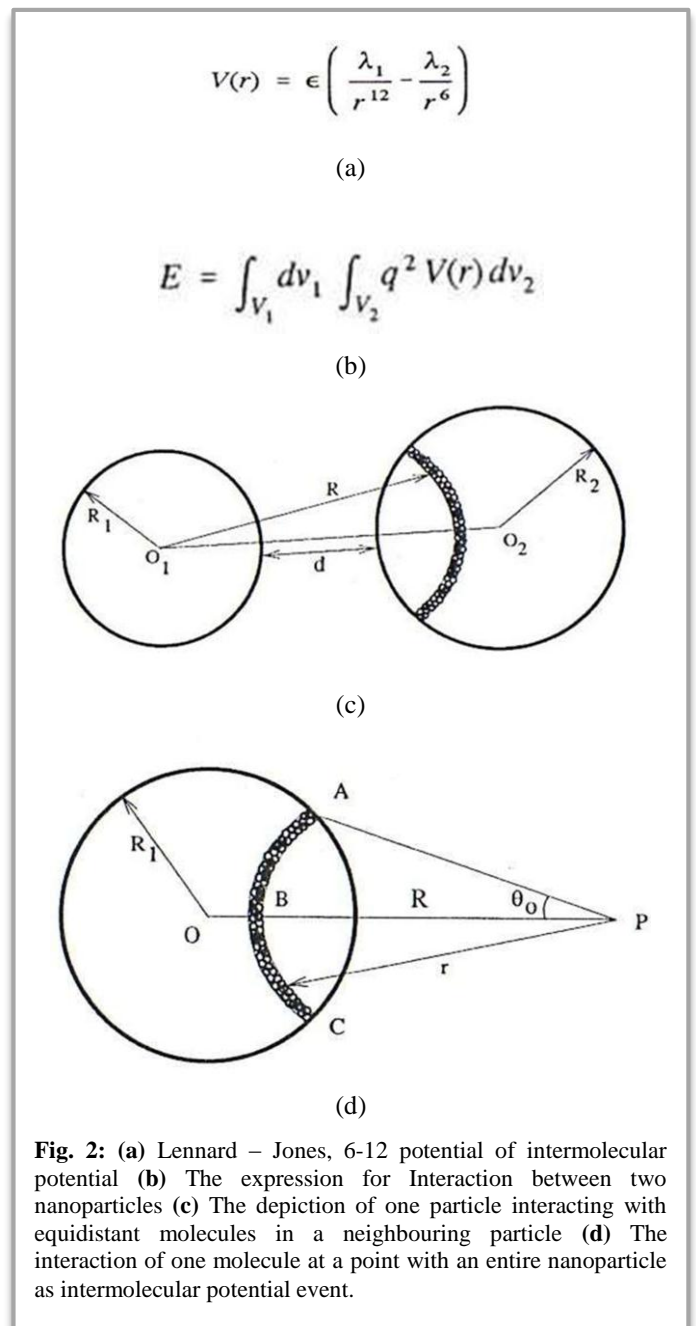


Fig. 2: (a) Lennard - Jones, 6-12 potential of intermolecular potential (b) The expression for Interaction between two nanoparticles (c) The depiction of one particle interacting with equidistant molecules in a neighbouring particle (d) The interaction of one molecule at a point with an entire nanoparticle as intermolecular potential event.

$$E(d) = \frac{16\lambda_1 q^2 \pi^2}{4725} \frac{d^{21}}{(2R+d)^{14} (4R+d)^7} \frac{1}{d^6} \left[\begin{aligned} &5.25 \times 10^2 \left(\frac{R}{d}\right)^6 + 1.60 \times 10^4 \left(\frac{R}{d}\right)^7 + 2.50 \times 10^5 \left(\frac{R}{d}\right)^8 + 2.33 \times 10^6 \left(\frac{R}{d}\right)^9 \\ &+ 1.5 \times 10^7 \left(\frac{R}{d}\right)^{10} + 7.1 \times 10^7 \left(\frac{R}{d}\right)^{11} + 2.56 \times 10^8 \left(\frac{R}{d}\right)^{12} + 7.23 \times 10^8 \left(\frac{R}{d}\right)^{13} + \\ &1.6 \times 10^9 \left(\frac{R}{d}\right)^{14} + 2.8 \times 10^9 \left(\frac{R}{d}\right)^{15} + 3.8 \times 10^9 \left(\frac{R}{d}\right)^{16} + 4.21 \times 10^9 \left(\frac{R}{d}\right)^{17} \\ &+ 3.5 \times 10^9 \left(\frac{R}{d}\right)^{18} + 2.15 \times 10^9 \left(\frac{R}{d}\right)^{19} + 9.27 \times 10^8 \left(\frac{R}{d}\right)^{20} + 2.49 \times 10^8 \left(\frac{R}{d}\right)^{21} \\ &+ 3.15 \times 10^7 \left(\frac{R}{d}\right)^{22} \end{aligned} \right] - \frac{\lambda_2 q^2 \pi^2}{d^3} \frac{6}{(4R+d)(2R+d)^2} \left[\begin{aligned} &(\ln(4R+d) - 2\ln(2R+d) + \ln(d)) \\ &\times \left(1 + 8\left(\frac{R}{d}\right) + 20\left(\frac{R}{d}\right)^2 + 16\left(\frac{R}{d}\right)^3 \right) + \\ &\left(4\left(\frac{R}{d}\right)^2 + 16\left(\frac{R}{d}\right)^3 + 8\left(\frac{R}{d}\right)^4 \right) \end{aligned} \right]$$

Fig. 3: The particle to particle potential relation based on molecule to molecule Lennard – Jones 6 -12 potential being obtained from analytical integration in Fig 2(b)

Radial Distribution Function (RDF)

Table 3: Radial Distribution Function(RDFs)- Particulate level for 27.5nm silica, SiO₂

	Peak1	Minimum1	Peak2	Minimum2	Peak3	Minimum3	Concentration of Suspension
Minimum/Peak Position	35nm	50nm	70nm	80nm	100nm	105nm	0.315 v/v
Minimum/Peak Height	2.2	0.45	1.4	0.8	1.1	0.9	
Minimum/Peak Position	40nm	60nm	75nm	95nm	-	-	0.200 v/v
Minimum/Peak Height	1.5	0.7	1.0	0.9	-	-	
Minimum/Peak Position	50nm	70nm	80nm	105nm	-	-	0.100 v/v
Minimum/Peak Height	1.2	0.85	1.0	0.95	-	-	

Table 4: Radial Distribution Function(RDFs) – Atomic/Molecular Level, SiO₂ –Vitreous silica

	Peak 1	Minimum1	Peak 2	Minimum2	Peak 3	Minimum3	Peak 4
Minimum/Peak Position	1.5	2.5	3.2	-	4.3	4.5	5.3
Minimum/Peak Height (Areal density of element at "r")	2000	1000	2500	-	6000	5500	8000
Bonding Atoms Species	Si-O	O-O	Si-Si	-	Si-O	O-O	Si-Si

While the RDFs were obtained with a single type of silica, SiO₂ sol, dispersed with deionized and/or deuterated water – the medium diluent were slightly varied, but after putting a drop of sol on carbon – coated grid it was completely dried, so on the TEM grid, there were only silica nanosilica nanoparticles of same size and chemistry but the interparticle distance, density on grid being related to initial sol suspension concentration variations, clearly proves that the RDFs change when interparticle distance alone changes while nothing else changes – hence the atom – bond organization theory and a new intermolecular force are clearly evident in amorphous nanoparticles of silica. Then nanoparticles of silica had a particle size 27.5 nm.

It says —"the exact form of interparticle potential is complex" and difficult to know it —"a priori". So we need an additional and/or alternative phenomenology, namely, —"the new intermolecular force and atom – bond organization theory".

When interparticle distance changes, the electron clouds can change on account of van der waals force i.e. VDW but the, their positions, distances & bond angles cannot change due to VDW which only affects electron clouds. So, it is a clincher of —Atom – Bond organization theory and a new intermolecular force in amorphous silica nanoparticle powder.

In bulk monolithic silica glass, it is a microsize material with uniform density and continuous mass system inside the volume of silica glass. So its atoms, bond angles cannot shift or change over vast length scales of μm-s or mm-s as it would not be continuous medium/material as we see in a microsize material. But in some silica as amorphous nanoparticles being a non-crystalline and also no vast distance of continuous mass it can shift atom positions, interatomic distances, bond angles at least to a small extent but the intermolecular force is very big and also new mechanism seen only in nanosize particles. This is the phenomenon of atom – bond organization theory and a new intermolecular force in amorphous silica, SiO₂ nanoparticles and nanopowder.

The RDFs show that repulsive forces are more as the concentration of nanoparticles increases. The MS Thesis research of Thirunavukkarasu Asaimuthu [4] obtained a particle – to – particle van der waals potential directly from molecule – to – molecule van der waals potential. When we fix the particle size R, the repulsive force depends directly on the repulsive term in the Lennard – Jones, 6 – 12 potential and attractive part depends on attractive term in the L – J, 6 -12 potential and attractive part depends on attractive term in the

L – J, 6 – 12 potential. So repulsion increases as the constant in repulsive term increases and the attraction depends on the attractive term depends on the attractive constant in L – J, 6 – 12 potential. But the repulsive term largely varies as 16th power of distance between nanoparticles while attraction varies as 3rd power of distance between particles.

At equilibrium, zero VDW energy, repulsive term and attractive term are equal. This equilibrium point has largest no. of nanoparticles at its interparticle distance so that maximum peak in RDF increases as the concentration of nanoparticles increases. So repulsion increases sharply with distance but attraction plays catch-up with repulsion slowly.

The equilibrium point is very sharp and intense in dilute solution of nanoparticle. But when concentration increases, the equilibrium point is less intense and flatter at and near the equilibrium potential zeropoint. The intermolecular force has strongly overpowered all the particles to place them at one equilibrium interparticle distance. Hence the intermolecular force is powerful enough to dominate particle - to – particle energy and distance with lower residual energy particles – nearly all nanoparticles are fixed at one particular equilibrium interparticle distance. But at higher concentration of particle in suspension, the interparticle distance increases but is also broader variation of interparticle distance still. So it is the repulsive part constant and attractive part constant in the L – J, 6 – 12 potential which also overpowers and dominates the particle – to – particle equilibrium distance for entire particle, not just scattering the values of distances between nanoparticles. It is now self – evident that the atom – bond organization theory and a new powerful long – range intermolecular force is seen in amorphous silica nanoparticles. The same silica at 53 μm silica has many orders of magnitude lower friction. Also, the water contact angle on amorphous silica is 20° more than crystalline silica – the atom – bond organization and new intermolecular force are so powerful – even in a thin surface film and even more in nanoparticle is highly evident [23]

Also silica of 53μm silica has orders of magnitude lower friction than nano silica [7].

The morphology of 53μm is not very vital being nearly spherical powder particle and it is intermolecular force of lower magnitude that sees a big decrease in friction.

In [23], thin film of amorphous silicon leads to a big increase in water contact angle by 20° even nearly to the maximum

value of 180° with amorphous spherical or so nanoparticle of silica, SiO_2 , it is bound to vindicate the atom – bond organization theory and a new Intermolecular force in this nanopowder.

The particulate RDFs show that repulsive forces increase and particle- to –particle distances increases even though concentration of particles in the solution is higher, this implies a more powerful long-range intermolecular force is functioning. The deuterium heavy water is decreasing and light water is increasing, So, the polar hydrogen bonding is increasing even when concentration is increasing. The ability of water medium to absorb van der Waals potential is decreasing- per molecule mass decreases but a small polarization in H_2O and D_2O is same. Unit volume to absorb fractional charge is increasing, unit volume no. of nanoparticles is also increasing. The concentration increases by three multiples but the medium's density also increases three multiples. But the polarization charge capacity of medium increases as charge per unit volume is more – the water polar charges is like a dielectric and number of H_2O per unit volume is more. So, the interparticle spacing i.e, RDF should show more attraction at smaller distance, but on the other hand the repulsion between silica nanoparticles is more the distance between silica nanoparticles is more. Hence, the intermolecular force is far higher. Thus we infer that the atom-bond organization theory and a new intermolecular force is clearly proved.

The difference between Van Der Waals – conventional VDW and the new Intermolecular force is clear. There are two things in a material/fluid:

- (i) The position of atoms at certain points in 3 –D spatial extent
- (ii) What species of atoms is there at each point where there is an atom present

If (i) & (ii) are fixed only electron cloud, bond changes, then it is Van Der Waals. London dispersion force is probably a time dependant variation of Van Der Waals force.

But this new intermolecular force happens when either of (i) and/or (ii) is not fixed, say bond angle changes or species and/or position of atoms is not strictly fixed by molecular structure or material structure, then it is the new intermolecular force and atom – bond organization theory. While DNA has a structure & it coils into a chromosome. But the bases CTAG are paired specifically but whether

—”A” is in this strand or “T” is in that strand or the opposite i.e. “T” is in this strand and —”A” is in that strand, this variability changes the atomic species (between —”A” & —”T” only) and also position of said atomic species this brings in the new Intermolecular Force.

In this new interatomic potential & force the relative positions of atoms, bonds and electron clouds, change repeatedly over time intervals, then it is new interatomic forces and potential.

Thus the significance of change in RDFs, say merely, due to change of interparticle distance while nothing else differs is a new Intermolecular force. The data in Table 3 and Table 4

provide the details of particle suspensions of nanosilica as well as Molecular RDF of microsilica, SiO_2 respectively.

Ultrahydrophobic performance and corrosion

Corrosion is a widespread and visible everywhere and different approaches are used for corrosion control and protection, such as paints, cathodic protection, etc., Ultrahydrophobic material prevents contact between metal and water drop, such as the Cassie state in Lotus, where water just rolls off as hydrophobic lotus surface has micro air pocket between lotus leaf and water drop. Due to lack of water ferrous and some other metals cannot corrode to oxide in the absence of water contact. The water will slide down and away instead of sitting as drops and corroding metal surfaces.

Basically there are two types of surfaces. Oils are hydrophobic with large amount of (CH) Hydrocarbon groups. The opposite is water it has hydrogen bond and (OH) groups which slightly polarize and attract other (OH) groups, this is water attracting or —”hydrophilic”.

The polarization in (OH) groups is based on Van Der Waals forces i.e. Intermolecular forces. When intermolecular forces are more the (OH) groups polarize more and over larger space lengths and dimensions of nearly water molecules or (OH) groups. The hydrophobic surface will repel water viz- there are tiny air pockets that separate water and the hydrophobic surface.

Hydrophobic action is directly based on intermolecular forces. It will attract all other hydrophobic molecules (Oils. CH groups) and repel all water drops and (OH) groups. Silica, SiO_2 in nanopowder form has very high intermolecular force. Inside a nanoparticle the amorphous solid will shift and adjust Si – O bonds and positions of —”Si” atoms and —”O” atoms, just like (CH) groups have no polarization in their bonds, so no polarization of Si – O bonds and atoms will take place. If a water drop with (OH) groups comes and nears Nano – silica, it cannot attract the silica, which does not polarize.

So water shrinks away and rounds up its own H_2O drop almost as a sphere and even not contact the ferrous material surface – there are micro air pockets between water and metal surface – the Cassie state in a lotus surface.

So water drops shrink away and polarize other water molecules in rain drop instead of trying to polarize the silica molecules in the nanoparticle. This is due to the new, high intensity intermolecular force in amorphous SiO_2 , silica nanoparticles i.e. because of SiO_2 nanoparticles to organize bonds and atoms position in amorphous nanoparticle of SiO_2 . Due to lack of water contact or lower area of water contact on metals such as steel corrosion is controlled and decreased to a large extent. The present industrial coatings are made of continuous layers of silica as opposed to spherical nanosilica in a medium which is then a coating of composite material on metal in a thin layer and water contact decreases and corrosion is less. The coating is superhydrophobic in particles of nanosize. Fig. 4, Fig.5 and Fig. 6 show the depiction of various levels and types of Hydrophobic and hydrophilic behaviour in solid surfaces.

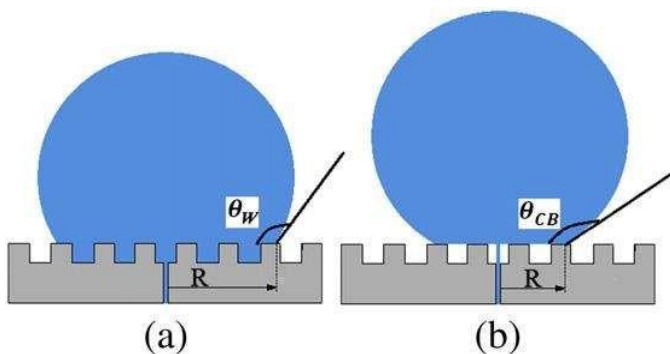


Fig. 4: Filling the liquid up to a rough surface through the solid substrate: (a) Homogeneous Wenzel fashion; (b) heterogeneous CB FASHION. R is the radius of the circular contact area between solid and liquid.

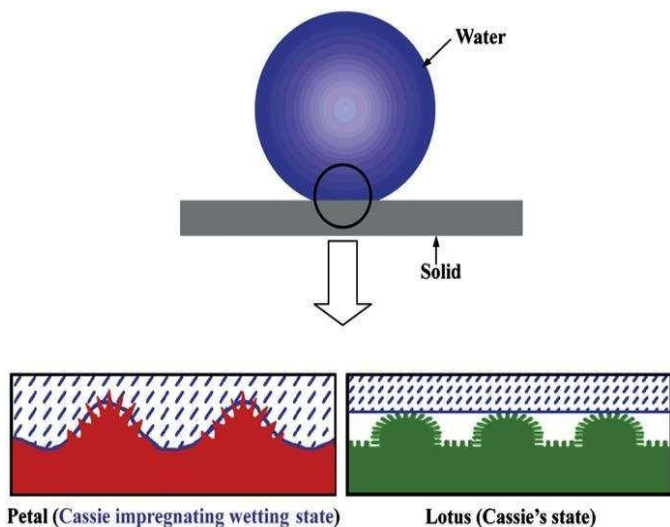


Fig. 5: Schematic illustrations of a drop of water in contact with the petal of a red rose (the Cassie impregnating wetting state) and a lotus leaf (the Cassie's state)

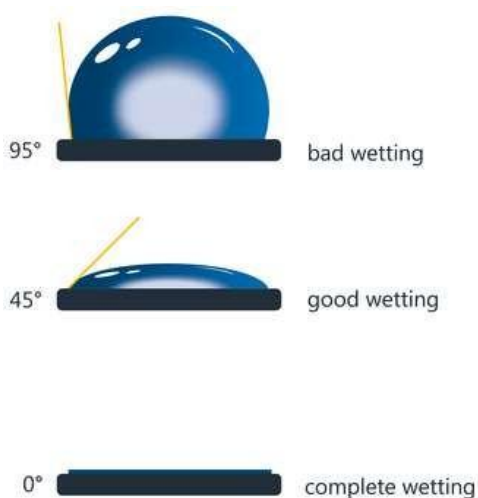


Fig. 6: Contact angle and wettability

water contact angle of amorphous silica based on intermolecular forces is :

$$\sigma_{ls} - \sigma_{gs} = \sigma_{ly} \cos(\theta)$$

σ_{ls} – surface tension at liquid solid interface, and σ_{gs} – surface tension at gas – solid interface, and σ_{lg} – surface tension at liquid gas interface, and $\cos(\theta)$ = water contact angle, θ cosine of it, and $\cos(\theta) = -1 + ((\Delta\rho/\sigma_{lg}) I)$

$$\Delta\rho = \rho_l - \rho_g$$

$$\sim 1 \text{ gm/cc for H}_2\text{O, and } I = \int V(z) dz$$

V is the Van Der Waals potential, and I is the integral of V

In the complete non- wetting limiting case , $\theta = 180$ degrees & $\cos\theta = -1$

$$\theta = 167.58^\circ$$

V(z) integral is integral of van der waals potential at minimum point of water above metal surface – also the top of intervening air pocket and integrate V, Van Der Waals potential from bottom minimum point – level of water to topmost point of water level- water drop point.

This is an advanced application of amorphous silica nanoparticle in corrosion control.

RESULTS AND DISCUSSION

We say liquid/even liquid crystals even though it just involves rearrangement of structure in crystallites but never at macroscopic scale and these are not at atomic molecular level right upto macro, rather lower length scale. We say gases, we also say a glass is a frozen liquid or is amorphous. All of these do not have a lattice structure, crystalline structure is absent – this new intermolecular force/potential bridges the divide between types of structures as well as states of matter, so our understanding is almost sweeping across all substances and materials. This research bridges large varieties and gaps in our understanding of materials and also substances with the potential for more advances – an unusual unification and generalization of disparate classes of materials and substances.

The SiO₂ glass especially melt processed liquid- it has —very high viscosity – high hardness and from low density liquid molten glass to relatively —more solid – substantive melt frozen glass and has one interatomic distance of highest probability in the —Radial distribution function(RDF). On the other hand —amorphous materials can be nucleation and growth – they either add-up or build-up from small to big size either in solid or liquid phases with various processing methods. It is a tiny phase and grows up to a material bulk scale by vast array of processing methods. Amorphous materials growing up from tiny dimension to bulk material afford a possibility of two or more local maxima in interatomic distances in the atomic/molecular RDF. Particulate RDF indirectly indicate the atomic RDF and interatomic potential to a minimum extent if not its full quantification.

The calculation of water contact angle is based on theoretical

Both glass and amorphous have less than full density i.e. packing of SiO_2 can be less than the most compact in crystalline version of the material. The new intermolecular force in materials functions by changing atom positions and bond angles in these materials, in less dense structure. It is an in-between phenomenon to bridge non-crystalline solids and fluid liquids and gases. Inside a silica nanoparticle the atom & bonds are –"fluid", can change and not –"frozen" even though the material does not change its volume and does not change its shape.

We have this new intermolecular force in amorphous nanopowders of silica(SiO_2). It is unique to amorphous nanopowder form and single molecular species constitution. This interatomic potential intermolecular force is an unusual, high power and long range force unique to above said nanopowder and can lead to unusual and even omnipresent applications such as ultrahydrophobic materials, imagine you can put this material everywhere there is water and/or corrosion on land based water, sea-going ships, a car windshield in rain, even in small water usage applications, even say tools in agricultural context, in construction structures, the list goes on and on, the idea that where there is water, we can -apply this new long-range intermolecular force.

We have amorphous nanopowder of silica(SiO_2) and being glassy, its atoms/molecules and the bonds i.e. interatomic bonds can change position of atoms (there is no 3D lattice) it can change bond angles and it is dynamic, the changes in atom positions and angles between bonds can repeat change, relax in response to water or in response nearby amorphous silica nanoparticles while at the same time the size and shape of the silica nanopowder particle does not change to a significant extent.

The inside of silica nanoparticle is sort of –"fluid" at atomic level but the size of and shape of the entire nanoparticle is fixed and does not change, the change in the inside of the nanopowder means the electron clouds can shift, reposition, rearrange with the long range response to the water and/or neighbour amorphous nanoparticle (the higher repulsion in high nanoparticle dose in solution means particle to particle equation Fig. 3, [4] shows particulate repulsion is directly related to atomic repulsion in L-J, 6-12 potential of interatomic potential equation - the power and spatial range of this intermolecular force and energy value of the interatomic potential from this phenomenon is large and powerful not seen in other intermolecular forces such as Van Der Waals or London Dispersion etc. this is a big feature of nanomaterial/nanotechnology not seen in other conventional materials. It even may mean that tertiary structure of DNA, the molecules in water, liquids and imagine gases they just consist of similar intermolecular forces, just that a nanoparticle in solid, with less no. of configurations of atoms and bonds while in liquids and gases the number of configurations of liquids and gases is much larger no of options for positions of constituent atoms/molecules but we are not treating those cases in this research as of now.

Once we state the new Intermolecular force, we derive a nanoparticle to nanoparticle potential between 2 spherical nanoparticles of silica(SiO_2) starting with molecule to

molecule Lennard – Jones 6-12 potential of two corresponding silica molecules in two nearby nanoparticles insides of Silica material make-up. This particle to particle potential is done by analytical integration in 3-dimensional coordinates of two nanoparticles of silica starting Lennard – Jones 6 – 12 intermolecular potential resulting in particle to particle potential.

Then we use the powder metallurgy compaction of silica nanopowders and find the friction forces. From friction, we find particle level forces between nanoparticles and its resultant friction forces at particle level, this comes from analysis of compaction forces in green compaction of nanopowders in silica.

The above calculation is at a static position of nanoparticles. But how do we show that position of atoms and bonds is actually shifting in this intermolecular force during compaction or when the density of green compact of nanosilica particles is increasing inside die cavity during compaction. So we obtain Radial Distribution function(RDF) of nanoparticle to nanoparticle is changing when a sol suspension of nanosilica changes and increases concentration of nanosilica, the particle to particle increases, but particle to particle repulsion is directly related to molecule to molecule repulsion and no attractive term of molecular attraction, hence we infer particle to particle behaviour is directly related to molecular potential only. The only change is average particle to particle distance, so the particle should change the molecular RDF inside the neighbour to neighbour particle or else the shift in RDF will be same for bulk silica VDW as well as nanoparticle VDW, but in this study is at least 20 orders of magnitude lower in bulk silica L-J, 6-12 interatomic potential. The molecules and structure are same but phenomenon is different and only way to explain is shift inside the nanoparticle's atoms and bonds and mechanism of electron clouds and London dispersion is similar in both nano and micro and atom bond organization is the only thing one can imagine in nanoparticle but can never happen in a microsize of micron size silica or monolithic silica. Also when density of green compact of nanosilica is increasing during PM compaction, the closeness of particles is increasing just like in a high concentration sol of silica, the closeness of silica nanoparticles is increasing and both increase repulsion forces and needs higher compaction forces which is manifested in friction of compaction being higher in nanoparticles. The change in particle to particle distances as RDF is without change in thermal parameters, hence it means at molecule level average thermal energy is same hence it must lead to change is position and bond angles i.e. atomic/molecular RDF inside Nanoparticle changes or else repulsion of particles due to conventional VDW cannot shift repulsion distances on a scale of Nanometers. The first peak is dominant at low sol concentration particulate RDF, but at higher concentration the distances of particle is not—"bunched" but it is —"spread out" with wide interparticle distance variations in sol. The shape of particulate RDF changes, not just position of peaks. Low intensity conventional VDW forces cannot work the particulates on a scale of many nanometers which the powerful Atom-Bond organization and new intermolecular force can achieve

We found the equilibrium inter-particle distance and then increased it by 1nm. So for an increase of 1nm distance more than minimum energy $V(r)_{\min}$, for nano – SiO₂ of say 1nm radius spherical particle, the decrease in intermolecular force is about half the decrease in intermolecular potential when compared to conventional Van Der Waals. So the intermolecular force in nanosilica is powerful as well as long-range. This is especially true since, the equilibrium distance between two 1nm particles is at a higher interparticle distance and for conventional VDW potential used for microsize silica, when same constants are used in 1nm particle calculation of minimum potential energy equilibrium distance, the energy minimum is at a smaller separation of molecules – here we assume Van Der Waals for micro as well as nano silica is same. So, the higher equilibrium distance in nano means both the repulsive and attractive terms in Lennard- Jones, 6-12 potential are more powerful and longer range in nanosilica when compared to same terms based on microsilica data, so, indeed this intermolecular force is powerful and long-range as compared to conventional VDW based on 53 μ m particles of amorphous silica powder materials.

While the absolute values of equilibrium energy is higher in the model of conventional VDW, it is so only because the equilibrium distance itself is smaller in conventional VDW, but when you move particles to a further 1nm higher distance, the decline is very rapid and severe in conventional VDW. But in the theoretical model based on direct Intermolecular force from simulation, the equilibrium is at a higher interatomic distance (the repulsive term is stronger), but at the same time increasing the interatomic distance away from the equilibrium point, the potential is higher intensity and it is a long range force compared to conventional VDW, this new intermolecular force is higher intensity as well as more of a long-range force when compared to micron material conventional VDW force/potential.

A new high – intensity and even long-range intermolecular force vis – a – vis existing intermolecular force is a valid finding. This is a high intensity force but only seen in amorphous nanopowders such as silica but only in nanoparticles with single atomic or single molecular species in the amorphous nanopowder. There are novel applications in day – to – day context such as corrosion and ultrahydrophobic performance. With their intensity and long range nature they have the potential in day – to – day and highly novel applications. The hydrophobic application can produce vast cost control, safe to use in existing areas and even corrosion and maintenance where corrosion is an area that figures in the entire GDP of emerging as well as established economies. New large innovative avenues must be created and implemented due to unique nature of this new Intermolecular force.

CONCLUSION

Atom – bond organization theory and a new high-intensity and long – range intermolecular force in amorphous single atomic/single molecular species nanopowders for novel and vast innovative applications such as Ultrahydrophobic materials for unique nature of this new intermolecular force is

established with strong and firm validation herewith.

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