QUANTUM STATES OF NANODIAMOND – PROTEIN INTERACTION

***A.A. Zimin*, I.A. Densov, P.I. Belobrov**

MOLPIT, Siberian Federal University, Institute of Fundamental Biology and Biotechnology, Institute of Biophysics SB RAS: Svobodny79, Krasnoyarsk, 660041, Russia

E-mail: reyenka@gmail.com; d.ivan.krsk@gmail.com; peter.belobrov@gmail.com

Nanodiamond shows unusually high affinity and specificity to proteins. This effect was first observed on rapid isolation of recombinant apoobelin from *Escherichia coli* [1]. However, quantum-mechanical explanation of the underlying precipitation mechanism is poorly understood. We suggest the basic explanation behind high nanodiamond – protein affinity based on the collective states of interacting electrons in diamond nanoparticles, water, and protein.

The concept of collective states has been widely used in theoretical investigation of metallic compounds, where overlap between "delocalized" non-bonding conduction band and "localized" bonding valence band occurs. When band gap is present, there is clear separation between the two, leading to the introduction of tight-binding approximation. Being extremely successful at large scale near-perfect crystals, tight-binding model should be extrapolated with great care to nanoscale dielectric particles.

We provide evidence for existence of collective electron bonding states in nanodiamond particles using both numerical integration of the Schrödinger equation on 1D one-particle Kronig-Penney potential model and *ab initio* investigations of ground-state wavefunctions morphology of diamondoids $C_{123}H_{100}$, $C_{211}H_{140}$ and $C_{302}H_{172}$ at DFT R-B3LYP level of theory with 6-31G(d,p) basis set in the GAMESS-US package. We also conclude from qualitatively identical behavior of 1D and *ab initio* models that foundation of the observed effect lay in the symmetry of the system and is unrelated to particular theory level. Several computations at HF level of theory with at least 6-31G(d,p) basis set were performed, showing qualitative invariance of the result. In order to take surface tension into account, we have deformed the particle non-uniformly from the surface, decreasing deformation gradually. This resulted in simultaneous presence of "deformed" and "perfect" regions in diamond molecule. We then have studied localization of the collective states. Deformation results in bonding states wavefunction localization shift from particle core to the subsurface layer.

We propose here a possible explanation for high protein – nanodiamond affinity. Similarity between sizes of nanodiamond and a typical globular protein (about 5 nm) allows us to suppose formation of the condensed phase with strong intermolecular interaction. However, *ab initio* simulations on that scale are nowadays hardly possible, and in order to obtain quantitatevely correct results they usually require large basis sets with diffuse additions and level of theory comparable

with CCSD(T) thus making computations unfeasible for large systems. Taking that into account, we introduce greatly simplified 1D Kronig-Penney model (Fig. 1). This figure shows on 1D model that it's not always possible to distinguish bonding states belonging to neighboring molecules: the definition of "molecule" probably should be revisited in case of molecular ensembles. We then conclude that when intermolecular interactions are considered, it's vital to take into account collective electron states. For example, even in relatively well-known case of ion hydration "cooperativity" plays important role [2], and structured region spans well beyond what is known as first or second hydration shell.

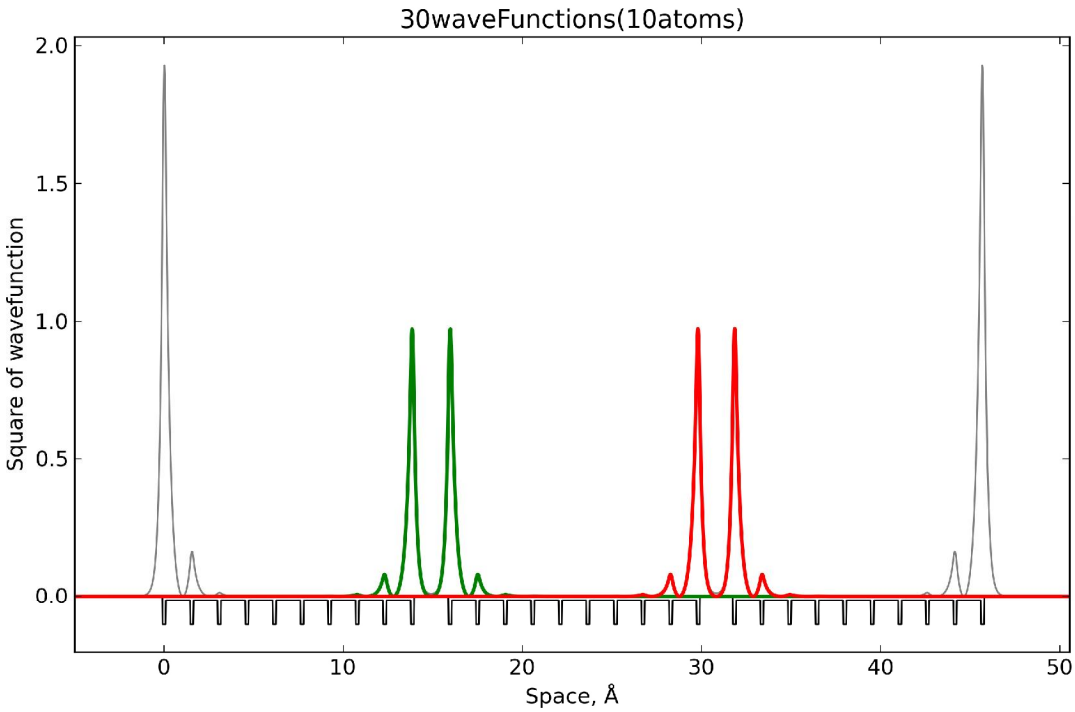

Figure 1. Two "HOMO's" for the three hypothetical ten-atomic 1D molecules show that collective bonding states are extremely important when considering intermolecular interactions. Computations are made using the Surface States Explorer application (freely available at our website http://molpit.com/?page=35).

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