



## SDI FINAL EVALUATION FORM 1.1

### PART 1:

Journal Name:	<a href="#">Physical Science International Journal</a>
Manuscript Number:	Ms_PSIJ_23370
Title of the Manuscript:	THE STUDY OF SILVER NANOPARTICLES IN BASIS OF SLATER FUNCTIONS
Type of the Article	Review papers9

### PART 2:

FINAL EVALUATOR'S comments on revised paper (if any)	Authors' response to final evaluator's comments
<p>1. Authors write "The descriptions of the problem is given in line 20-23". It is not descriptions of the problem. Authors must say what problems with silver particles are. What properties of them are not clear till now? Why did they study the 16-atomic silver? May be has it some remarkable properties but is not studied enough? The paper needs to have a real Introduction.</p> <p>2. Authors write: "The shape of Ag<sub>16</sub> nanoparticles is considered as a sphere..." Why? They must find the shape of nanoparticles from the calculations (finding the minimum of energy). There are some published works where it is said that the Ag-16 cluster has a flat shape (<a href="#">Solid State Communications Volume 144, Issues 3-4</a>, October 2007, Pages 174-179), a deformed sphere <a href="http://www.genetical.com/dc/ScientificResearch/Thesis/4Chapter4/chapter4.html#Spherical">http://www.genetical.com/dc/ScientificResearch/Thesis/4Chapter4/chapter4.html#Spherical</a> Approximation), an ikosahedron capped with three atoms (arXiv:physics/9908034v1 [physics.atm-clus] 18 Aug 1999). So, the shape is a problem.</p> <p>3. Authors take the formulae for the size of the Ag nanoparticle stated in the cited work [4] for colloid particles, but they use it for quantum calculations. However, the colloid model is phenomenological and gives only an order of quantities. Authors must find the size (as well as a shape) of nanoparticles from the calculations.</p> <p>4. Authors write: "The visual model of nanoparticles Ag<sub>16</sub> was established and the cartesian coordinaties of atoms were calculated in molecular coordinate system". What means "The visual model of nanoparticles Ag<sub>16</sub> was established"? Authors must obtain coordinates of atoms in the process of their calculations.</p> <p>4. Authors ignored my previous remark about explanations: why they use the semi-empirical WH method. Semi-empirical methods use usually for large systems when ab initio methods can not work. For 16-atomic particles ab initio methods work very well and give much more correct results than semi-empirical. I do not see any reason to use a semi-empirical method for 16-atomic particles. If authors prefer to use the semi-empirical method they must fulfill test calculations (for example, for Ag<sub>2</sub>) and compare results with known ab initio data.</p> <p>5. Authors must to include other published data in the text and to discuss comparison. (Data for Ag-16 are here: <a href="http://www.general-ebooks.com/read/15462646">http://www.general-ebooks.com/read/15462646</a>).</p>	<p>The purpose of the work is to learn the possibility of Slater functions in theoretical study of nanoparticles. If the stability is provided, the calculations can be carried out for any Ag<sub>n</sub> nanoparticles.</p> <p>The shape is a problem, and the authors used sphere shape assumptive.</p> <p>The formula (1) is not used in the quantum mechanical calculations. It is used to determine the number of atoms in given size of nanoparticles, and for the construction of the model of the nanoparticles.</p> <p>By using the constructed model it is possible to find out the coordinates of atoms. The quantum mechanical calculations can be carried out if the coordinates of the atoms are known.</p> <p>Usually Gauss functions are used in the ab initio methods. In the work authors used the Slater functions.</p> <p>Agree.</p>