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## **SDI FINAL EVALUATION FORM 1.1**

### PART 1:

Journal Name:	Physical Science International Journal
Manuscript Number:	Ms_PSIJ_23370
Title of the Manuscript:	THE STUDY OF SILVER NANOPARTICLES IN BASIS OF SLATER FUNCTIONS
Type of the Article	Review papers

### PART 2:

FINAL EVALUATOR'S comments on revised paper (if any)	Authors' response to final evaluator's comments
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? My be has it some remarkable properties but is not studied enough? The paper needs	
to have a real Introduction.	
2. Authors write: "The shape of $Ag_{16}$ 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 (Solid State Communications Volume 144, Issues 3–4, October	
2007, Pages 174–179), a deformed sphere	
http://www.genetical.com/dc/ScientificResearch/Thesis/4Chapter4/chapter4.html#Spherical	
Approximation), an ikosahedron capped with three atoms (arXiv:physics/9908034v1	
[physics.atm-clus] 18 Aug 1999). So, the shape is a problem.	
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.	
4. Authors write: "The visual model of nanoparticles $Ag_{16}$ was established and the cartesian	
coordinaties of atoms were calculated in molecular coordinate system".	
What means "The visual model of nanoparticles $Ag_{16}$ was established"? Authors must	
obtain coordinates of atoms in the process of their calculations.	
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 Ag2) and	
compare results with known ab initio data.	
5. Authors must to include other published data in the text and to discuss comparison.	
(Data for Ag-16 are here: <u>http://www.general-ebooks.com/read/15462646</u> ).	

### **Reviewer Details:**

Name:	Anonymous
Department, University & Country	Institute of Materials Science, Federal Agency of Science Organizations, Russia

