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# Analysis of silver four-atom cluster interaction with the surface of silicon dioxide by density functional theory

© **Tatiana I. Isaak**,[1]* **Daria O. Martinova**,[1] and **Oleg Kh. Poleshchuk**[2+]
[1] *National Research Tomsk State University. Lenin Pr., 36. Tomsk, 634050. Russia.*
*Phone: +7 (909) 546-63-06. E-mail: taina_i@mail.ru*
[2] *National Research Tomsk State University. Lenin Pr., 30. Tomsk, 634050. Russia.*
*Phone: +7 (913) 829-14-54. E-mail: poleshch@tspu.edu.ru*

*Supervising author; +Corresponding author

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**Abstract**

The calculations were carried out of some silver and silicon-containing molecules in the gas phase with the use of density functional theory using the all-electron basis set DGDZVP in the software package GAUSSIAN'03 and TZ2P+ of the Amsterdam density functional program. It is shown that silicon oxide with a high probability can be reacted with silver cluster. The calculated ESCA levels and the natural bond orbitals indicate the significant interaction between the virtual orbitals of silver atoms.