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Comment on "Study of the Interaction of a Palladium Nanocontact with a Hydrogen Molecule"

[A. L. Klavsyuk et al., *JETP Letters* 93, 530 (2011)]

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The authors of the commented work formulated a number of urgent problems on the effect of impurities on the atomic structure and mechanical properties of a palladium nanocontact. However, a number of questions arise primarily about the method of study used. In particular:

(i) The authors wrote, "In order to model the formation of metallic nanocontacts, we used the method of molecular statistics with many-particle potentials [13]." Then, the potential used by the authors was presented. It is noteworthy that the form of a part of the repulsive-interaction potential from the work W. Zhong, Y. Cai, and D. Tomanek, Phys. Rev. B **46**, 8099 (1992) cited in the commented work as [13] differs from that used in the commented work. As a result, it is unclear how the authors used the parameters of the potentials from [13]. If the form of the potential was changed after certain mathematical transformations, this problem (as well as the applicability of the parameters from [13] and the effect of these transformations on the accuracy of the reproduction of the physical phenomenon under study) was not discussed.

(ii) From qualitative reasons, it can be assumed that the binding energy for one-dimensional nanocontacts will be higher than that for the same atoms on a surface. (Although the applicability of this approach to calculate surface configurations can sometimes be doubtful, see, e.g., Phys. Rev. B **61**, 2203 (2000).) However, the authors did not present any results of ab initio calculations that can confirm the correctness of the used parameters of the potential for the calculations of the properties of the surface configurations and the one-dimensional nanocontact.

(iii) The so-called tight-binding approach used in the commented work was developed and used primarily for the calculations of the properties of metallic nanostructures with fcc lattices. The authors of the commented work did not present the results of test calculations that confirm the applicability of this approach for the description of H–H bonds.

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