

Reply to ‘Comment on “Structural characterization, reactivity, and vibrational properties of silver clusters: A new global minimum for Ag₁₆”’ by P. V. Nhat, N. T. Si, L. V. Duong and M. T. Nguyen, Phys. Chem. Chem. Phys., 2021,23, DOI: D1CP00646K

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Abstract

Recently, P. V. Nhat et al., have discussed and commented on our article (DOI: 10.1039/D0CP04018E) for the case of the most stable structure of Ag₁₅. They have found a new most stable structure (labeled as 15-1) in comparison to the putative global minimum reported by us, which is a four layered 1-4-6-4 stacking structure with a C_{2v} point group (15-2). In this reply, we have performed a larger structure search which allowed us to confirm the results of Nhat et al. The results show the existence of multiple isoenergetic isomers with similar structure motifs for the Ag₁₅ system, increasing the problem complexity to locate the global minimum. The results in regard to the structure and electronic properties of the new lowest energy structure are discussed. © the Owner Societies 2021.