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A comparative study of oxygen-doped and pure beryllium clusters based on structural, energetic and electronic properties

Jin-Ye Li, Di Wu, Ying Li*, Zhi-Ru Li

Institute of Theoretical Chemistry, Laboratory of Theoretical and Computational Chemistry, Jilin University, Changchun 130023, China

ABSTRACT

The lowest-energy structures of the oxygen-doped Be_n (n = 1–12) clusters are obtained at the B3PW91 level. Various energetic and electronic properties of the Be_nO clusters are systematically investigated using the QCISD(T) method, which are compared with those of pure Be_{n+1} clusters. The evolution of these properties with cluster size shows the unique stability of $Be_{11}O$, which can actually be considered as an ionic compound $(Be_{11})^{2+}O^{2-}$. On the one hand, O^{2-} has 8 valence electrons, satisfying the octet rule. On the other hand, the Be_{11}^{2+} moiety has a shell-closed electronic configuration, which renders itself particularly stable.

Keywords: Be_n cluster, dopant, theoretical study, density functional theory, stability

* Corresponding author
E-mail address: liyingedu@jlu.edu.cn (Y. Li)