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

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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 $(\text{Be}_{11})^{2+}\text{O}^{2-}$. 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)

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