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Determination of ground state structures of selected medium-sized clusters via first-principles global search JIJUN ZHAO, Dalian University of Technology — Due to the existence of numerous local isomers on the potential energy surface, determining the most stable structures of medium-sized clusters is one of the most challenging tasks in cluster physics. Recent years, we have explored the potential energy surface of medium-sized clusters using first-principles calculations combined with global search methods like genetic algorithm and simulate annealing. The examples on a few selected examples such as B_{80}/B_{101}, $Na_{1-3}Si_{1-11}$, and $(WO_3)_{2-12}$ clusters will be briefly illustrated. The size-dependent electronic properties of these clusters will also be discussed and compared with available experimental data.

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