Performance of modified Lennard-Jones potential to seed ab initio calculations of small cadmium clusters

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Weakly bonded Cadmium clusters have, even for small number of atoms, many isomers that are stable structures. Before any attempt to use ab initio calculations on these clusters, a limited set of good possible stable isomers (seeds) has to be defined. It is customary to use Lennard-Jones isomers as seeds in weakly bonded clusters. Here we show how a simple extended Lennard-Jones (ELJ) potential performs better than Lennard-Jones potential. We find that ELJ clearly decreases the size of possible stable isomers and increases its fitness. We also assess the capability of ELJ potential to predict isomers of Cd3 to Cd10 that coincide or are close to actual ab initio structural-optimized isomers.