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Structural and electronic properties of aluminum nanoclusters MRUDULA RAPARLA, TUNNA BARUAH, RAJENDRA R. ZOPE, University of Texas at El Paso — The electronic properties of Al clusters containing upto 60 atoms are investigated using an all electron density functional theory using large polarized Gaussian basis sets with 39 Gaussians per atom (NRLMOL basis). We have performed an extensive search for the lowest energy isomers for clusters up to Al_{21}. We build a database of candidate structures for the ground state using different strategies. First, a few structures are randomly generated and fully relaxed using plane wave pseudo potential method. We also performed simulated annealing runs using ab initio molecular dynamics for clusters upto Al_{20}. In three sets of simulated annealing runs the clusters were heated upto 900 and 1000K and were slowly cooled to 50K at different rates. After every half picosecond, the cluster was quenched. Additionally the best basin hopping geometries obtained using empirical embedded atoms potential were also fully optimized. The process generates 40-50 structures for each size. All the structures are relaxed using full-potential PAW method using a large energy cutoff. For larger clusters we used best available geometries from literature obtained from basin hopping and simulated annealing techniques. The electronic properties of Al clusters are subsequently determined for this database at the all-electron level using Gaussian basis set.

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