

Electronic and structural properties of sodium clusters: A pseudopotential based density functional approach

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We present rigorous, *ab initio* calculations for structural and electrical properties of Na clusters. Our calculations, which combine pseudopotentials with a gradient-corrected density functional, allow for a greatly reduced computational load at no inherent loss of accuracy. We have applied this approach to the study of the dependence of Na cluster polarizability on cluster size, up to 20 atoms. At $T=0$, we reproduce the salient qualitative features of the experimental curve. At a finite temperature, we find that the modified cluster structure accounts for most of the quantitative discrepancy between theory and experiment.