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Adaptive Tempering Monte Carlo Optimization of Calcium Clusters.[1] X. DONG, E. BLAISTEN-BAROJAS, School of Computational Sciences, George Mason University, Fairfax, VA 22030 — The global minimum energy structures of calcium clusters with 15 to 34 atoms were obtained by the Adaptive Tempering Monte Carlo (ATMC) method. The cluster binding energy was obtained within a tight binding approach with parameters reported in previous work[1]. The ATMC optimization process is fast and drives the system across configuration space very effectively reaching the global minimum within a small number of tempering events. The structure of six cluster sizes 15, 16, 18, 21, 23 and 25 corresponding to the global minimum has not been reported in the literature for any other metals. Three clusters Ca_{15}, Ca_{21} and Ca_{23} are relatively more stable than the others in this size range. Melting of these clusters are further studied with the weighted histogram analysis method and the free energy profile is predicted. The melting transition is monitored with a novel structural order parameter that reflects the mobility of surface atoms, their bonding order and bonding directionality. [1] X. Dong, G. M. Wang, E. Blaisten-Barojas, Phys. Rev. B 70, 205409 (2004).

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