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Bond Stiffening in Small Clusters, and its Consequences SHOBHANA NARASIMHAN, RAGHANI PUSHPA[1], UMESH WAGHMARE, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India — We have used density functional theory and density functional perturbation theory to compute the interatomic force constant tensors for small clusters of Si, Sn and Pb; these results have important implications for the size dependence of the elastic and thermal properties of nanosized objects. We find a clear sequence of relationships: as the size of the cluster is decreased, bonds get shorter and stiffer and vibrational frequencies higher; however the behaviour relative to the bulk depends on the coordination number of the latter. Though all the clusters we have studied are softer than the corresponding bulk, vibrational amplitudes may be enhanced or damped relative to the bulk values, and vary non-monotonically with size. Scaling relations connect results for varying sizes and different elements. These results also provide a framework for understanding recent results showing that, surprisingly, some clusters have melting temperatures that are much higher than that of the corresponding bulk material.

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