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Confinement effects on the vibrational properties of colloidal quantum dots PENG HAN, GABRIEL BESTER, Max Planck Institute for Solid State Research — We present a first-principles study of the confinement effects on the vibrational properties of colloidal III-V and II-VI nanoclusters with thousand atoms and radii up to 16.2 Å. We describe the connection between the vibrational properties including surface-optical and -acoustic modes, coherent acoustic modes and the structural changes induced by the surface. We highlight the qualitative difference between III-Vs and II-VIs. We can clearly ascribe most of the observations to the large relaxation of the clusters dominated by an inward relaxation of the surface penetrating deep inside the cluster in case of the III-Vs and a large distribution of bond length at the surface of II-VIs. These strong confinement effects tend to disappear for clusters with more than 1000 atoms, where a small red shift of the Raman peaks remains, due to a softening in response to undercoordination. The coherent acoustic phonons are identified and found to be in good agreement with results from the Lamb model and experiment. We explain why the simple model by Lamb gives an accurate description in case of the breathing modes while the vibrational properties of small NCs are poorly described by continuum models in general.

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