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Probe new crystal structures using static and dynamical simulations

Recently, based on the development of accurate theoretical approaches for calculating energies of assemblies of atoms and computing power, together with the progress in searching methodologies, numerous successful predictions have been obtained. In this talk, I will introduce some of ourrecent work on crystal structure predictions using a static approach, ab initio random structure searching (AIRSS) and dynamical method called ab initio metadynamics. At the end, we will also introduce some results on the vibrational spectroscopy of liquids by ab initio molecular dynamics simulations.

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Alvin Van Valkenburg

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Photograph by Xiaodong Hu