

Institute for Materials Science Universität Stuttgart

Colloquium **Materials** Science Summer Semester 2020

"Oscillatory dynamics in simple systems at elevated temperatures beyond a perturbational treatment of anharmonicity,

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Abstract

The importance of anharmonicity for describing fundamental materials properties,

starting from finite heat conductivity due to phonon-phonon scattering, can hardly be overemphasized. For crystalline matter, the principal microscopic gauge is constituted by the broadening in energy of the phonon dispersions, corresponding to q-dependent phonon lifetimes.

Here the case of elemental AI at temperatures up to the melting point will be considered. Experimental data obtained by inelastic neutron scattering will be compared to calculations of q-dependent line broadenings on the basis of density-functional theory. While the standard approach of perturbation theory gives significant discrepancies, the agreement with spectra computed by ab initio molecular dynamics is satisfactory [1]. Further, an analysis of the atomic interaction constants will show how to construct numerically efficient phenomenological potentials that accurately reproduce anharmonic properties as computed by DFT at very small computational effort, and finally the limitations of perturbation-derived linewidths will be elucidated.

[1] A. Glensk et al., Phys. Rev. Lett. 123, 235501 (2019)

Meeting number: 121 018 7422 Meeting password: ptCXcMuH333

Meeting link: