Lattice Dynamics of the Iron Pnictides: Real-time Collaboration between Theory and Experiment

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With tight schedules and limited time available for inelastic x-ray scattering studies, one needs to ensure that allocated time is used as efficiently as possible. On-site dedicated theoretical/computational support can be valuable in this regard. Using only the atomic species and positions as input, modern *ab initio* calculations can accurately calculate the phonon dispersion and related quantities for a large number of systems. By calculating the inelastic structure factor at any Q, these calculations are beneficial in both planning the experiment and analyzing the results. Moreover, differences between the measured data and theoretical calculations can help identify important new physics driving the properties of novel correlated systems. We have used such calculations to better and more efficiently measure the phonon dispersion and elastic constants of several iron pnictide superconductors. By discussing these experiments, we hope to demonstrate the advantages of on-site theoretical support.

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