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New spectroscopic approaches for periodic systems SANDRA LUBER, University of Zurich — Knowledge about local properties is extremely helpful for the analysis of structures and interactions. Moreover, it is a valuable source of information for the characterisation of dynamic processes and facilitates the interpretation of experimental data. In case of vibrational spectroscopy, for example, it is desirable to determine the impact of certain atoms/molecules on the bands in the experimental spectra. This may be straight forward for small systems but becomes more and more complex for larger systems. Calculations provide additional insight allowing the targeted study of specific structures. In this way, it is possible to quantify the contributions of, for instance, solute and solvent molecules [1] or adsorbates on solids. We present novel, computationally efficient methods for the calculation of properties for periodic systems such as liquids and solids. These are applied to calculate, among others, vibrational spectra via ab initio molecular dynamics [2,3]. References: [1] S. Luber, J. Phys. Chem. A 117 (2013) 2760. [2] S. Luber, M. Iannuzzi, J. Hutter, J. Chem. Phys. 141 (2014) 094503. [3] S. Luber, submitted.

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