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**Phonon Calculations Using the Real-Space Multigrid Method (RMG)** JIAYONG ZHANG, WENCHANG LU, EMIL BRIGGS, NC State University, YONGQIANG CHENG, A.J. RAMIREZ-CUESTA, Oak Ridge National Lab, JERRY BERNHOLC, NC State University — RMG, a DFT-based open-source package using the real-space multigrid method, has proven to work effectively on large scale systems with thousands of atoms. Our recent work has shown its practicability for high accuracy phonon calculations employing the frozen phonon method. In this method, a primary unit cell with a small lattice constant is enlarged to a supercell that is sufficiently large to obtain the force constants matrix by finite displacements of atoms in the supercell. An open-source package PhonoPy is used to determine the necessary displacements by taking symmetry into account. A python script coupling RMG and PhonoPy enables us to perform high-throughput calculations of phonon properties. We have applied this method to many systems, such as silicon, silica glass, ZIF-8, etc. Results from RMG are compared to the experimental spectra measured using the VISION inelastic neutron scattering spectrometer at the Spallation Neutron Source at ORNL, as well as results from other DFT codes. The computing resources were made available through the VirtuES (Virtual Experiments in Spectroscopy) project, funded by Laboratory Directed Research and Development program (LDRD project No. 7739)

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