Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-principles modeling of resonant Raman scattering for the understanding of phonons and electrons in nanomaterials[1] LIANGBO LIANG, Oak Ridge National Laboratory, VINCENT MEUNIER, Rensselaer Polytechnic Institute, JIA-AN YAN, Towson University, BOBBY SUMPTER, Oak Ridge National Laboratory — Raman spectroscopy is a popular tool that can probe both phonons and electrons of the materials. First-principles modeling is important in aiding the understanding of experimental data. Raman modeling is typically based on the classical Placzek approximation and limited to the non-resonant condition, and thus the laser energy dependence of Raman intensities could not be captured. Here we showed that resonant Raman scattering could be captured by upgrading the classical approach, i.e., by calculating the dynamic dielectric tensor at the laser energy instead of the commonly used static value at zero energy. Our method was successfully applied to recently synthesized atomically precise graphene nanoribbons, and revealed the photon-energy-dependent Raman intensity of the radial breathing like mode (RBLM), which explained experimental observations that RBLM can be only observed in certain laser energies. Additionally, we also explored anisotropic 2D material, ReS2, and found that the angle-resolved Raman polarization dependence of its Raman modes is sensitive to the laser energy, as confirmed by recent experiments. The intricate electron-phonon coupling could lead to no simple rule for using Raman polarization dependence to determine the crystalline orientation.

[1]LL is supported by Eugene P. Wigner Fellowship at Oak Ridge National Laboratory and CNMS (a DOE Office of Science User Facility).

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Date submitted: 02 Nov 2016 Electronic form version 1.4