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Abstract for an Invited Paper
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Electron-phonon coupling from finite displacements: including electron correlation and higher order terms¹
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The band gap is a central quantity determining many excited-state phenomena of materials, such as their optical properties. The effects of electron correlation on the band gap have been thoroughly investigated for some time, but the effects of electron-phonon coupling, which are fundamental for the study of temperature dependent properties, have received less attention. I will present recent developments in the study of electron-phonon coupling using the finite displacement method^{2,3} that allow us to study electron-phonon coupling beyond semilocal density functional theory and also including terms beyond the lowest order in the interaction. To illustrate the new approach, I will present three examples. First, I will describe the calculation of the temperature dependence of band gaps in semiconductors and insulators using the *GW* method.⁴ Second, I will discuss temperature induced band inversions in topological insulators, a description of which requires the inclusion of the spin-orbit interaction in the calculation of electron-phonon coupling.⁵ Third, I will show that higher-order terms in the electron-phonon interaction must be included for an accurate description of electron-phonon coupling in perovskite solar cell materials.

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²J.H. Lloyd-Williams and B. Monserrat, PRB **92**, 184301 (2015)

³B. Monserrat, PRB **93**, 014302 (2016)

⁴B. Monserrat, PRB **93**, 100301(R) (2016)

⁵B. Monserrat and D. Vanderbilt, arXiv:1608.00584 [cond-mat.mtrl-sci]