Abstract Submitted
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Large Scale GW Calculations Including Electron-Phonon Interactions[1] RYAN MCAVOY, Institute for Molecular Engineering, University of Chicago, MARCO GOVONI, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago; Materials Science Division, Argonne National Laboratory — Including the effect of electron-phonon coupling in first principle electronic structure calculations is crucial for the accurate prediction of band-gaps and temperature dependent carrier lifetimes. We present results for the electronic properties of condensed and molecular systems, including electron-phonon coupling, obtained by merging GW calculations [1] of eigenvalues and an efficient implementation of the Fan-Migdal-Debye-Waller self-energy. Our implementation does not require summation over virtual states and inversion of large dielectric matrices. Advantages of the algorithm presented here over standard techniques and its scalability will be discussed. [1] Govoni, Marco, and Giulia Galli. "Large scale GW calculations." *Journal of chemical theory and computation* 11, no. 6 (2015): 2680-2696.

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