Abstract Submitted
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Plasmon Pole Approximations within a GW Sternheimer implementation VINCENT GOSSELIN, MICHEL COTE, Univ of Montreal — We use an implementation of the GW approximation that exploits a Sternheimer equation and a Lanczos procedure to circumvent the resource intensive sum over all bands and inversion of the dielectric matrix. I will present further improvement of the method that uses Plasmon Pole approximations to evaluate the integral over all frequencies analytically. A comparison study between the von Linden-Horsh and Engel-Farid approaches for energy levels of various molecules along with benchmarking of the computational ressources needed by the method will be discussed.

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