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Plasmon Pole Approximation within the GW Lanczos approach VINCENT GOSSELIN, BRUNO ROUSSEAU, MICHEL COTE, Univ of Montreal — The well-known DFT gap problem is adressed by computational methods that are more ressource intensive both in terms of memory and time requirements. Amongst other methods, the GW approach has known great success in the field of electronic structure calculations. Addressing the main bottlenecks impeding one shot GW calculations, a sum over all conduction states and an integral over all frequencies must be carried. Within an implementation of the GW method based on the Lanczos algorithm, the sum over conduction states is treated with a Sternheimer method whereas the frequency integral is carried out numerically. In this talk, I will present an implementation of a plasmon-pole model combined with the Lanczos method that allows a treatement of this integral that is computationally favorable.

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