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The G0W0 band gap of ZnO: effects of plasmon-pole models GABRIEL ANTONIUS, University of Montreal, MARTIN STANKOVSKI, DAVID WAROQUIERS, ANNA MIGLIO, Universite Catholique de Louvain, HEMANT DIXIT, University of Antwerpen, KIROUBANAND SANKARAN, MATTEO GIANTOMASSI, XAVIER GONZE, Universite Catholique de Louvain, MICHEL COTE, University of Montreal, GIAN-MARCO RIGNANESE, Universite Catholique de Louvain, UNIVERSITY OF MONTREAL TEAM, UNIVERSITE CATHOLIQUE DE LOUVAIN TEAM, UNIVERSITY OF ANTWERPEN TEAM — Carefully converged calculations are performed for the band gap of ZnO within the G0W0 approximation. The results obtained using four different well-established plasmon-pole models are compared with those of explicit calculations without such models (the contour-deformation approach). We evaluate the difference between plasmon-pole models that enforce the f-sum rule and those that are fitted to reproduce the low energy response. In the case of ZnO, plasmon-pole models enforcing the f -sum rule underestimate the low-frequency region of the dielectric function probably because of the presence of semi-core states in these calculations. Our results confirm that the band gap of ZnO is underestimated in the G0W0 approach as compared to experiment.

Gabriel Antonius
University of Montreal

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