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Band structure of polyethylene from many-body perturbation theory ARIEL BILLER, Weizmann Institute of Science, Israel, SAHAR SHARIFZADEH, Lawrence Berkeley National Laboratory, USA, LIOR SEGEV, Weizmann Institute of Science, Israel, SOHRAB ISMAIL-BEIGI, Yale University, USA, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory, USA, LEEOR KRONIK, Weizmann Institute of Science, Israel — The electronic structure of polyethylene is an important benchmark and the infinite chain limit for the electronic properties of many molecules, monolayers, and oligomers. Therefore, the band structure of the ideal, one-dimensional polyethylene chain has been extensively researched, from both the experimental and the theoretical viewpoints. Despite this extensive effort, to the best of our knowledge agreement between theoretical calculations and the electronic structure obtained from photoelectron spectroscopy could only be obtained using artificial shifting and "stretching" of the computed data. Here, we present a quantitative quasi-particle band-structure for polyethylene using many-body perturbation theory. The approach is employed within the G_0W_0 approximation, based on a starting point calculated within the generalized gradient approximation to density functional theory. We compare our calculated band-structure to angle resolved photoemission spectroscopy measurements for various long saturated carbohydrates, demonstrate a much improved agreement with experiment, and discuss remaining discrepancies and their possible origins within both theory and experiment.

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