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Amorphous carbon for photovoltaics FRANCESCA RISPLENDI, JEFFREY C. GROSSMAN, Massachusetts Inst of Tech-MIT, Materials Science and Engineering dept. — All-carbon solar cells have attracted attention as candidates for innovative photovoltaic devices. Carbon-based materials such as graphene, carbon nanotubes (CNT) and amorphous carbon (aC) have the potential to present physical properties comparable to those of silicon-based materials with advantages such as low cost and higher thermal stability.In particular a-C structures are promising systems in which both sp^2 and sp^3 hybridization coordination are present in different proportions depending on the specific density, providing the possibility of tuning their optoelectronic properties and achieving comparable sunlight absorption to aSi. In this work we employ density functional theory to design suitable device architectures, such as bulk heterojunctions (BHJ) or pn junctions, consisting of a-C as the active layer material.Regarding BHJ, we study interfaces between aC and C nanostructures (such as CNT and fullerene) to relate their optoelectronic properties to the stoichiometry of aC. We demonstrate that the energy alignment between the a-C mobility edges and the occupied and unoccupied states of the CNT or C_{60} can be widely tuned by varying the aC density to obtain a type II interface.To employ aC in pn junctions we analyze the p- and n-type doping of a-C focusingon an evaluation of the Fermi level and work function dependence on doping.Our results highlight promising features of aC as the active layer material of thin-film solar cells.

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