Abstract Submitted
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Absolute potential of the Fermi level of single-walled carbon nanotubes via hydrogenase complex formation.[1] TIMOTHY MCDONALD, DRAZENKA SVEDRUZIC, YONG-HYUN KIM, JEFFREY BLACKBURN, SHENGBAI ZHANG, PAUL KING, MICHAEL HEBEN, National Renewable Energy Lab — The absolute potential of the Fermi level of nanotubes as a function of nanotube type is not presently understood, and is important for many nanotube applications and sorting strategies. Here, we study complexes of recombinant [FeFe] hydrogenases and single-walled carbon nanotubes. We find evidence that novel charge-transfer complexes are formed and are stable, which enables further study and application of this system. The hydrogenase functions as a hydrogen electrode sensitizing the nanotubes to the redox half-reaction for hydrogen. Thus the potential can be altered by changing the molecular hydrogen concentration, and this tunability is utilized to bleach various semiconducting nanotube transitions. By observing which are bleached and which remain emissive, we determine the alignment of the potential of the Fermi level of semiconducting single-walled carbon nanotubes. The experimentally determined Fermi level alignment is confirmed theoretically by the first-principles DFT-PBE method.

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