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Photovoltaic effect for narrow-gap Mott insulators

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Solar cells, based on conventional band-semiconductors, have low efficiency for conversion of solar into electrical energy. The main reason is that the excess energy of the photon absorbed by an electron/hole pair beyond the band-gap becomes heat through electron-phonon scattering and phonon emission; through these processes electrons and holes relax to their band edges within a characteristic time scale of the order of $10^{-12} - 10^{-13}$ secs. We will discuss that a narrow-gap Mott insulator can produce a significant photovoltaic effect and, more importantly, if appropriately chosen it can lead to solar cells of high efficiency. In this case, a single solar photon can produce multiple electron/hole (doublon/hole) pairs, an effect known as impact ionization, faster than other relaxation processes such as relaxation through phonons. It has been proposed previously that this process could lead to an efficient solar cell using band-gap semiconductors; however, the characteristic time-scale for impact ionization is comparable to that for electron-phonon relaxation in band-gap semiconductors. The reason that a Mott insulator can behave differently is that the large Coulomb repulsion present in a Mott insulator leads to a large enhancement of the impact ionization rate. Provided that this enhancement does occur in an appropriately chosen Mott insulator, it can be demonstrated that the efficiency can improve significantly over conventional band-insulators. At present, we are doing calculations on specific transition-metal-oxide based materials believed to be Mott-insulators using extensions of the density functional theory (hybrid functionals) in combination with many-body perturbation theory. Our goal is to determine a promising candidate with suitable band structure and transition matrix elements leading to fast transition rates for impact ionization to occur in a time-scale faster than other relaxation processes.