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Condensed Matter Physics Issues in Inorganic Photovoltaics

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This talk will identify some of the outstanding fundamental issues and research opportunities in inorganic PV that, in my view, condensed matter physicists could help solve. These include: (1) Understanding what limits the introduction of electrons or holes (“doping”) into semiconductors and finding how to overcome such bottlenecks. The fact is that, with very few exceptions, most semiconductors can be doped either by holes (e.g. tellurides and antimonides) or by electrons (e.g., some oxides and arsenides) but not by both (one notable exception is Si). This PV-limiting factor has been recently understood to reflect an intrinsic tendency of semiconductors to develop “anti-bodies” (i.e., spontaneously generated defects that negate the deliberately introduced carriers) in response to added free-carriers. (ii) Understanding the rare coexistence of optical transparency with electric conductivity. Indeed, “Transparent Conductors” are required in both organic and inorganic PV solar cells, but designing them and making them is limited by our current understanding of such seemingly contradictory phenomena. (iii) The need to *systematically* search (or even design) new PV-enabling materials and nanostructures which overcome the current bottlenecks. Such bottlenecks include the need to avoid rare (e.g. In) or toxic (e.g., Cd) elements and, most importantly, avoid materials that manifest light-induced metastabilities (e.g., DX-like centers) which “pin” the Fermi level. The role of first-principles theory of defects in quantitatively predicting such behavior, and of “Inverse Design” in surveying astronomic spaces in search for the material with desired target properties will be discussed.

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