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Inorganic Alloys and Nanostructures for Photovoltaics[1]

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Semiconductor alloys and nanostructures are often used as photovoltaics materials and building blocks. In this talk, I will present results using large scale ab initio calculations to study the electronic structures and optical properties of semiconductor alloys and nanosystems. First, I will discuss the results of GaN:ZnO alloy, its atomic structures and electronic properties. GaN:ZnO is an unconventional locally nonstoichiometric alloy. A special model Hamiltonian is developed to describe its configuration total energy and to study its atomic structure. We found that GaN:ZnO forms a homongeneous alloy with strong short range order at high temperature. Such short range order has big effect on its band structure and band edge electron states. The second system to be discussed is ZnTe:O. In this alloy, the O atoms induce an intermediate band within the ZnTe band gap. This can be used for intermediate band solar cell. The change of this intermediate band as a function of the O centration will be discussed. The theoretical solar cell efficiency calculated based on the optical absorption spectra between different bands is 63%. The other aspects of the material in order to reach such high efficiency will be discussed. Finally, I will present results of exciton binding energies in heterojunction nanostructures (e.g., nanorods or wires), especially for CdSe/CdTe and ZnO/ZnS nanorods. We found large exciton binding energies in such nanostructures at the interface. The implication of such large exciton binding energy and its effect on solar cell efficiency will be discussed.

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