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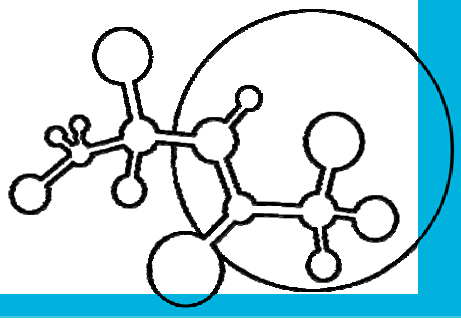

Quantum Efficiency Seminar and Colloquium

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Segregation and defect structures in CIGS solar cell absorbers

The chalcopyrite semiconductors CuIn1-xGaxSe2 (CIGS) and CuInSe2 (CIS) are excellent materials for high efficiency and low cost thin-film solar cells. This is due to the effective absorption of the solar spectrum and the inherent resilience to defects and composition fluctuations. Although the CIGS and CIS material in solar cells is highly inhomogeneous and exhibits a lot of different defects, the cell efficiencies are exceptionally high. If single crystalline absorbers are used, efficiencies are lower. Therefore, studying spatial inhomogeneities and defect structures is of great importance for understanding what supports and what diminishes the efficiency and robustness of the cells. We have employed Monte Carlo (MC) simulations based on density functional theory (DFT) to investigate spatial inhomogeneities, disorder phenomena and stoichiometries in CIGS and CIS materials. For CIGS systems we have studied the temperature-dependent, spatial In-Ga distribution. The simulations show that two phases coexist in thermal equilibrium below room temperature. Only at higher temperatures, CIGS becomes more and more a homogeneous alloy. A larger degree of inhomogeneity for Ga-rich CIGS persists over a wide temperature range, which contributes to the comparably low efficiency of Ga-rich CIGS solar cells. For the CIS material we have studied order-disorder phenomena and the stoichiometry of Cu-poor structures. It is known that Cd, diffusing from the CdS buffer into the Cu-poor CIS phases at the absorber-buffer interface, has an important beneficial impact on the cell efficiency. We have used DFT calculations and ab initio molecular dynamics to investigate the behavior of Cd in a Cu-poor phase. The aim of these studies, together with our search for alternative buffer materials, is the avoidance or reduction of Cd in chalcopyrite solar cells.

Date: **Tuesday, May 31st, 2011 4:15 pm**

Location: **FRIAS Seminar Room, Albertstr. 19, Freiburg**

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