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Dissertation press release 17.06.2019

Alkali metal treatment improves the efficiency of CIGS thin film solar cells

Title of the dissertation	Improving Cu(In,Ga)Se2 solar cell absorbers based on atomic-level modeling
Contents of the dissertation	In order to provide affordable and sustainable energy for the future, solar cells with high conversion efficiency are needed. The efficiency of thin film chalcopyrite solar cells has increased remarkably in recent years. Current efficiencies for converting energy of the solar radiation into electricity surpass 23,3%. The light harvesting absorber material in chalcopyrite solar cells is Cu(In,Ga)Se2 that can be used in thin film solar cells thanks to its high absorption of sunlight. In the case of Cu(In,Ga)Se2 cells, the recent considerable improvements were obtained when the cells were treated with alkali metals. The aim of this dissertation is to understand the effect of native point defects and alkali metal impurities on the atomic and electronic structure of the Cu(In,Ga)Se2 absorber layer. Experiments indicate that light (Li, Na) and heavy (K, Rb, and Cs) alkali metal atoms have different effects. Light alkali metal atoms mostly contribute by increasing p-type conductivity, open-circuit voltage, and fill factor, while heavy alkali metal treatment improves the surface morphology and further improves solar cell parameters. According to the present calculations, these effects arise from the tendency that the light alkali metal atoms prefer to accumulate on the Cu sublattice as impurities, whereas incorporation of heavy alkali metal atoms contributes mostly by phase separation.
Field of the dissertation	Engineering Physics
Doctoral candidate	Maria Malitckaya, M.Sc.
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Opponent	Prof. Dr. rer. nat. Karsten Albe, Technische Universität Darmstadt, Germany
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A doctoral dissertation is a public document and shall be available at Aalto University, School of Science's notice board in Konemiehentie 2, Espoo at the latest 10 days prior to public defense.