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**Atomic structure and interfacial energy of copper and cuprous oxide forming heterojunctions with the ZnO(0001) surface**[1] OLIVER WARSCHKOW, KATAWUT CHUASIRIPATTANA, MATTHEW LYLE, School of Physics, The University of Sydney, BERNARD DELLEY, Paul-Scherrer-Institut, CATHY STAMPFL, School of Physics, The University of Sydney — The system Cu/ZnO is industrially important as a catalyst for methanol synthesis and water-gas-shift reactions. The pairing of copper and zinc oxide is crucial to catalytic efficacy; however, the atomic-scale interactions between the two phases are far from resolved. This presentation will focus on three heterojunctions of relevance to catalytic action, namely, Cu(111):ZnO(0001), $Cu_2O$(110):ZnO(0001), and $Cu_2O$(111):ZnO(0001). We use density functional theory to characterize these interfaces in terms of their environment-dependent structure and energetics. This allows us to assess the relative stability of competing structures, and discuss their possible roles in an active catalyst.

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Oliver Warschkow
School of Physics, The University of Sydney

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