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SPECTROSCOPIC DISENTANGLEMENT OF THE QUANTUM STATES OF HIGHLY EXCITED COPPER DIMERS

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HCI D2, 4.00 pm

Project Summary: Both for high-resolution spectroscopy and ab initio quantum chemistry, the high density of states in excited transition metal systems was always an insurmountable obstacle. In this work, we demonstrate how to overcome this for small molecules by conducting the spectroscopy on the individual rotational quantum state of the individual isotopologue. Inspired by the extensive use of di-copper centers in nature, we chose the copper dimer as our sample. Building a novel laser ablation metal cluster source, we were able to produce the copper dimer in pulses of sufficient number density to apply non-linear, double-resonant spectroscopy on a molecular beam. For the low-lying electronic states, we could observe an additional spin-orbit state and could contribute to the first accurate ab initio calculations in this range. In the deep UV, we revisited dense, odd-shaped bands, which were so far reported to be impossible to assign. Preselecting the rotational quantum states, these bands decomposed into a rich network of bright and perturbing dark states. This first quantitative characterization of such states and their interactions reveals the complex nature of transition metal systems: nonadiabatic coupling of covalent and ion-pair states is ubiquitous and, already for a light period 4 element like copper, spin-orbit coupling cannot be neglected. While this sets the conceptual foundation for a variety of new experiments, it also provides a data set to calibrate respectively test new computational approaches to get a grip on transition metal systems and, thereby, to finally open a rational pathway towards green chemistry.

CV. Martin Beck obtained a diploma degree in physics (Dipl.-Phys.) from University of Konstanz in 2013. After finishing some projects, he started his doctoral studies in the van Bokhoven group in 2014. The experimental work was done under supervision of Dr. Peter Radi at PSI.