POTENTIAL CURVE OF GROUND STATE Cu_2 UP TO 98% OF THE DISSOCIATION ENERGY

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We report on an experimental and theoretical investigation of the ground electronic potential of dicopper. By taking into account our recent deperturbation study of the high lying energy map,[a] gateway levels are identified that allow access to vibrational levels of the ground state up to $\approx 98\%$ of the dissociation limit. Rotationally resolved two-color resonant four-wave mixing spectra (TC-RFWM) are analyzed by applying the 'near-dissociation expansion' (NDE) introduced by Le Roy.[b]

In addition to the determination of D_e, an accurate potential energy function is obtained to assess the structural and dynamical properties of this important transition metal species. *Ab initio* computations at the multi-reference configuration-interaction level of theory shed further light on the bound characteristics of this diatomic molecule.

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[a] Beck, M., P. Bornhauser, Bradley Visser, G. Knopp, J. A. van Bokhoven, and P. P. Radi. Nature Communications, 10(2019)3270

[b] Le Roy, Robert J. Journal of Quantitative Spectroscopy and Radiative Transfer, 186(2017)197