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Highly frustrated quantum magnetism in the mineral azurite: multi-step approach from first-principles computations to experimental data HARALD O. JESCHKE, INGO OPAHLE, ROSER VALENTI, Institut fuer Theoretische Physik, Goethe-Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany, HENA DAS, TANUSRI SAHA-DASGUPTA, Satyandranath Bose National Centre for Basic Sciences, Kolkata 700098, India, MICHAEL LANG, Physikalisches Institut, Goethe-Universitaet Frankfurt am Main, 60438 Frankfurt, Germany, SHIJIE HU, XIAOQUN WANG, Department of Physics, Renmin University of China, Beijing 100872, China, ROBERT PETERS, Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan, ANDREAS HONECKER, Institut fuer Theoretische Physik, Georg-August-Universitaet Goettingen, 37077 Goettingen, Germany — The natural mineral azurite $Cu_3(CO_3)_2(OH)_2$ is a frustrated magnet displaying unusual and controversially discussed magnetic behavior. We perform a theoretical study based on density functional theory as well as state-of-the-art numerical many-body calculations [1]. We propose an effective generalized spin-1/2 diamond chain model which provides a consistent description of experiments: low-temperature magnetization, inelastic neutron scattering, nuclear magnetic resonance measurements, magnetic susceptibility as well as new specific heat measurements. With this study we demonstrate that the balanced combination of first principles with powerful many-body methods successfully describes the behavior of this frustrated material.
[1] H. O. Jeschke *et al.*, Phys. Rev. Lett. **106**, 217201 (2011)

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