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Microscopic simulation and analysis of a spin crossover transition HARALD O. JESCHKE, L. ANDREA SALGUERO, ROSER VALENTI, Institut fuer Theoretische Physik, Universitaet Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany, BADIUR RAHAMAN, TANUSRI SAHA-DASGUPTA, S.N. Bose National Centre for Basic Sciences, JD Block, Sector 3, Salt Lake City, Kolkata 700098, India, CHRISTIAN BUCHSBAUM, VOLODYMYR PASHCHENKO, MARTIN U. SCHMIDT, Institut fuer Anorganische und Analytische Chemie, Universitaet Frankfurt, Max-von-Laue-Str. 7, 60438 Frankfurt, Germany — In spin crossover materials, an abrupt phase transition between a low spin state and a high spin state can be driven by temperature, pressure or illumination. Of a special relevance are Fe(II) based coordination polymers where, in contrast to molecular systems, the phase transition shows a pronounced hysteresis which is desirable for technical applications. A satisfactory microscopic explanation of this large cooperative phenomenon has been sought for a long time. The lack of X-ray data has been one of the reasons for the absence of microscopic studies. In this work, we present an efficient route to prepare reliable model structures and within ab initio density functional theory analysis and effective model considerations we show that in polymeric spin crossover compounds magnetic exchange between high spin Fe(II) centres is as important as elastic couplings for explaining the considerable cooperativity and thus the width of the hysteresis.

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