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Computational studies of the Fe(II) spin crossover compound $Fe[H_2B(pz)_2]_2(bpy)$[1] YIFENG CHEN, MARCO BUONGIORNO NARDELLI, Department of Physics, North Carolina State University — Using calculations from first principles, we studied the electronic and transport properties of the Fe(II) spin crossover (SCO) compound $Fe[H_2B(pz)_2]_2(bpy)$. The magnetic transition has been imposed by constrained magnetization calculations and the computed electronic structure agrees with available experimental data. Besides the characterization of the single molecule, we constructed a ?-stacking molecular chain of the compound and evaluated electronic transport in the direction of the chain for both the low-spin and the high-spin configurations. We found the high-spin configuration to be more conductive than the low-spin case, in agreement with experimental measurements of corresponding currents through disordered thin films. Molecule-molecule interactions are taken into account by the London dispersion forces. The spin-switchable electronic transport properties of this kind of Fe(II) SCO compound systems provide viable proofs for future switchable molecular spintronic devices and applications.

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Yifeng Chen
Department of Physics, North Carolina State University

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