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First-principles calculations of the magnetic interactions in Fe dimers[1] SERGEY STOLBOV, RICHARD A. KLEMM, TALAT S. RAHMAN, Kansas State University — We present the results of first-principles calculations of the magnetic interactions between the Fe(III) ions in Fe2 dimers, and those within the larger Fe8 cluster which interact by superexchange through two oxygen ions. The magnitude and sign of interaction is found to be strongly dependent on the Fe-O-Fe angle θ. We rationalize the obtained behavior analyzing the valence charge and spin densities calculated versus the angle. For the experimentally relevant range $100 \leq \theta \leq 105^{\circ}$, in addition to the sign and magnitude of the isotropic Heisenberg exchange interaction constant, we obtain the intramolecular global and local spin anisotropy interaction constants.

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