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First-principles study of magnetic interactions in monolayer FeSe
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of Wisconsin, Milwaukee — Due to its high-temperature superconductivity, the
monolayer FeSe has received considerable attention. Although long-range magnetic
order has not been observed, magnetic interactions among local moments of Fe
may play important role in the superconducting mechanism. Based on the density-
functional theory (DFT) calculations, a large number of magnetic configurations
are explored by using supercell and reciprocal-space approaches. Spin models for
the monolayer and bulk FeSe, which reasonably account for the DFT results, are
constructed.

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