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Spin polarization at the interface of LaMnO3 and Si heterostructure HUIPING ZHU, Nanjing University, GUOPING ZHANG, Indiana State University, XIAOSHAN WU, Nanjing University — Spin injection at a ferromagnet-semiconductor interface is one of the promising ways to add new functionality to the conventional devices. Here we study the spin injection from ferromagnetic LaMnO3 to semiconductor Si using first-principles calculations. We use two different methods: (1) Changing the distance between Si and LaMnO3 layers and (2) introducing the dimerization at the first Si layer. We find that when we reduce the distance between Si and LaMnO3 layer, both the total spin moment and the spin polarization at the Fermi-level change. There is a general trend that a stronger spin moment corresponds to a weaker spin polarization, but they do not follow exactly this trend at each distance. For the Si dimerization case, when the distance between the two Si atoms is reduced, the total spin moment increases whereas the spin polarization at the Fermi-level is not. Our results indicate that Si atoms with a smaller total spin moment may have a stronger spin polarization at the Fermi-level, and vice versa. Since the electrons at the Fermi-level play a key role in transport, the spin polarization at the Fermi-level, therefore, is more important than the total spin moment for spin injection.

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