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Highly Efficient (Cs_8V) Superatom based Spin-polarizer SHASHI KARNA, US Army Research Laboratory, APG, MD, HAIYING HE, RAVINDRA PANDEY, Michigan Tech, Houghton, MI, JOSE REVELES, SHIV KHANNA, Virginia Commonwealth University, Richmond, VA — Quantum transport through molecules and the possibility to manipulate spin has generated tremendous excitement. Here, we demonstrate unusual spin transport through a molecule of two Cs_8V magnetic superatoms. Calculations based on density functional theory and non-equilibrium Green's function methods find a much higher current for the spin-down charge carriers relative to the spin-up carriers in the model Au-(Cs_8V)-(Cs_8V)-Au device system with almost 100% spin polarization, indicating a highly efficient spin polarizer. The new behavior is rooted in strong coupling of the localized magnetic core on V and the itinerant electrons of the Cs shell atoms leading to nearly full spin-polarization.

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