Transport and thermoelectric properties of magnetic organic structures

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We analyze magnetic, transport and thermoelectric properties of narrow carbon polymers and magnetic organic chains, which are chemically functionalized with nitroxide (NO) groups. Numerical calculations of the electronic band structure and the corresponding transmission function are based on the Density Functional Theory. We predict that magnetic organic chains appear to be half-metallic ferromagnets with notable energy gap between spin-up and spin-down channels. This suggests that a device based on such structures could act as a very effective spin filter and its polarization may be changed with use of the gate voltage. Our calculations also predict very good thermoelectric performance of both types of organic structures, as the conventional and spin Seebeck coefficients are remarkably enhanced.

These results suggest that the studied magnetic organic structures would have a great potential for applications in spintronic devices.