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Novel One-Dimensional Organometallic Half Metals: Vanadium-Cyclopentadienyl, Vanadium-Cyclopentadienyl-Benzene, and Vanadium-Anthracene Wires LU WANG, Physics Department, Peking University, ZIXING CAI, JUNYU WANG, JING LU, GUANGFU LUO, LIN LAI, JING ZHOU, RUI QIN, ZHENGXIANG GAO, DAPENG YU, GUANGPING LI, WAI NING MEI, STEFANO SANVITO, PHYSICS DEPARTMENT, PEKING UNIVERSITY COLLABORATION, SICAS CENTER, LEE HALL, SUNY ONEONTA COLLABORATION, PHYSICS DEPARTMENT, UNIVERSITY OF NEBRASKA AT OMAHA COLLABORATION, PHYSICS DEPARTMENT, TRINITY COLLEGE DUBLIN COLLABORATION — By using the density functional theory, we find that organometallic multidecker sandwich clusters V2n+1Cp2n+2, Vn(FeCp2)n+1 (Cp = cyclopentadienyl), and V2nAnt$n$+1 (Ant = anthracene) may have linear structures, and their total magnetic moments generally increase with the cluster size. The one-dimensional (VCp)∞, (VBzVCp)∞ (Bz = benzene), and (V2Ant)∞ wires are predicted to be ferromagnetic half-metals, while the one-dimensional (VCpFeCp)∞ wire is a ferromagnetic semiconductor. The spin transportation calculations show that the finite V2n+1Cp2n+2 and Vn(FeCp2)n+1 sandwich clusters coupled to gold electrodes are nearly perfect spin-filters.

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