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Semiconducting (Half-Metallic) Ferromagnetism in Mn(Fe) Substituted Pt and Pd Nitrides SAMIR MATAR, ICMCB-CNRS, Université de Bordeaux, France, VOLKER EYERT, www.materialsdesign.com — Using first principles calculations as based on density functional theory, we propose a class of so far unexplored diluted ferromagnetic semiconductors and half-metals. Here, we study the electronic properties of recently synthesized *4d* and *5d* transition metal dinitrides. In particular, we address Mn- and Fe-substitution in PtN_2 and PdN_2. Structural relaxation shows that the resulting ordered compounds, $Pt_{0.75}(Mn,Fe)_{0.25}N_2$ and $Pd_{0.75}(Mn,Fe)_{0.25}N_2$, maintain the cubic crystal symmetry of the parent compounds. On substitution, all compounds exhibit long-range ferromagnetic order. While both $Pt_{0.75}Mn_{0.25}N_2$ and $Pd_{0.75}Mn_{0.25}N_2$ are semiconducting, Fe-substitution causes half-metallic behavior for both parent materials.

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