Physical Properties of alloys of two dimensional magnetic $Ni_xMn_{1-x}PS_3$

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Resumen

The transition-metal chalcogenophosphates MPX_3 exhibit magnetic ordering even at the limit of two dimensions. Specifically, $MnPS_3$ is a 2D Heisenberg-like antiferromagnet material [1] and their band gap and band edge positions, under a biaxial strain and electric field, are ideal for water splitting applications [2].

Based on experimental routes for the controlled replacement of Mn by Ni atoms, and by means of first principles calculations, in this contribution we will explore the magnetic and electronic properties of the monolayer of $Ni_xMn_{1-x}PS_3$. The exchange of the magnetic ion, for another with a partially unfilled *d* shell, have deep implications in both magnetism and chemistry.

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Referencias

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