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Supplementary

Transition Metal-Hyperdoped InP Semiconductors as Efficient Solar Absorber Materials

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Table S1. Crystal Structure of TM (TM = Ti, V, Cr, Mn), In and P atoms.

Atom	Space Group	Unit cell parameters
In	123	$a = b = 3.25$ Å $c = 4.95$ Å $\alpha = \beta = \gamma = 90^{o}$
Ti	187	$a = b = 2.95$ Å $c = 4.69$ Å $\alpha = \beta = 90^{o}$ $\gamma = 120^{o}$
V	221	$a = b = c = 3.03$ Å $\alpha = \beta = \gamma = 90^{o}$
Cr	221	$a = b = c = 2.91$ Å $\alpha = \beta = \gamma = 90^{o}$
Mn	217	$a = b = c = 8.92$ Å $\alpha = \beta = \gamma = 90^{o}$
P	2	$a = 7.86$ Å $b = 5.50$ Å $c = 11.26$ Å $\alpha = 73.38^{o}$ $\beta = 90.53^{o}$ $\gamma = 71{,}62^{o}$

Experimental data take from: https://periodictable.com/Properties/A/CrystalStructure.an.wt.html.

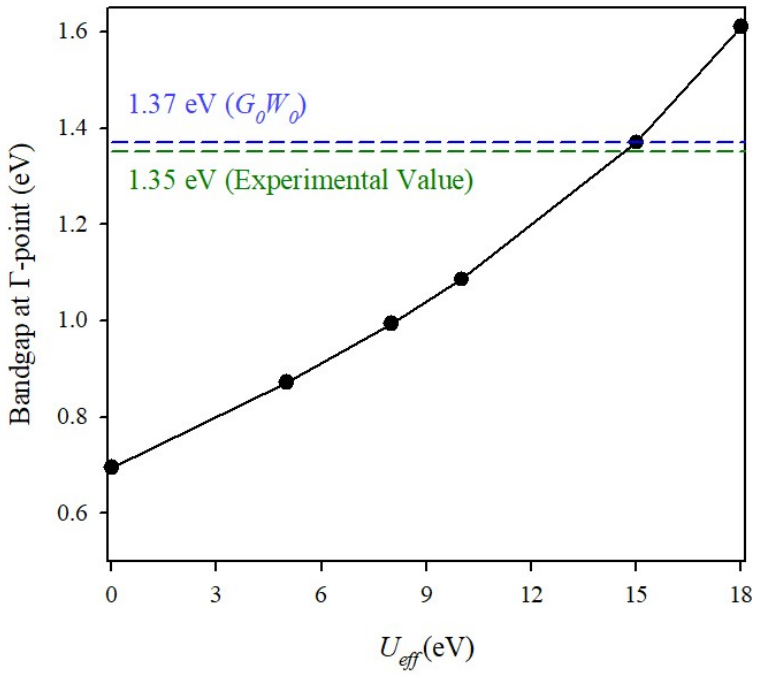

Figure S1. Calculated bandgap at Γ-point for InP by using PBE+*U* formalism (U_{eff} = 5, 8, 10, 15, 18 eV). Crystal structure optimizations were performed using the PBEsol. Blue and green dotted lines stand for G_0W_0 and experimental value.

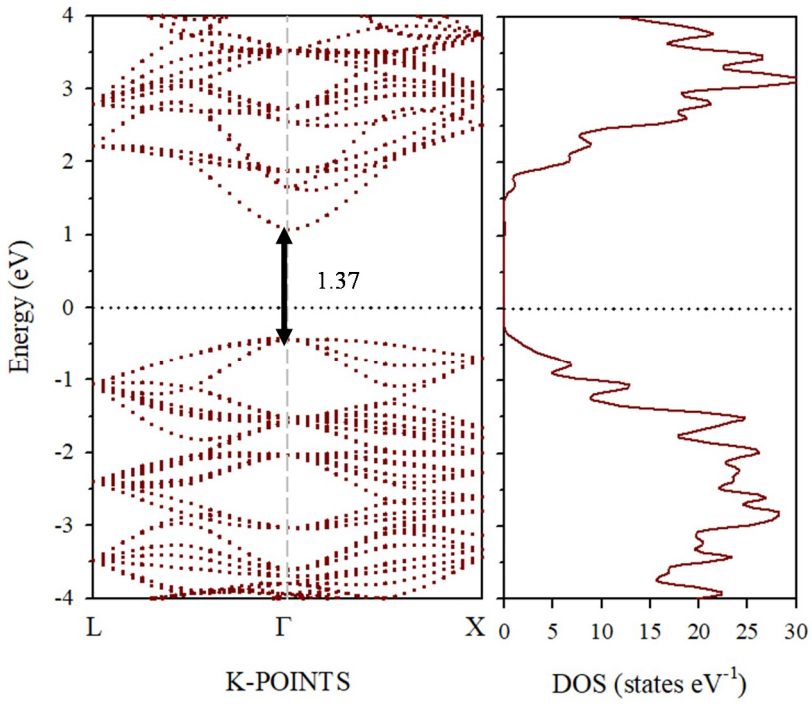

Figure S2. Electronic band structure (left) and Density of States (right) of InP calculated within G_0W_0 approach along to main energy differences at Γ-point. The zero energy has been set to the Fermi level (black dotted line). Spin-up and spin-down bands and DOS are not given separately as both contributions are the same for the native InP material.

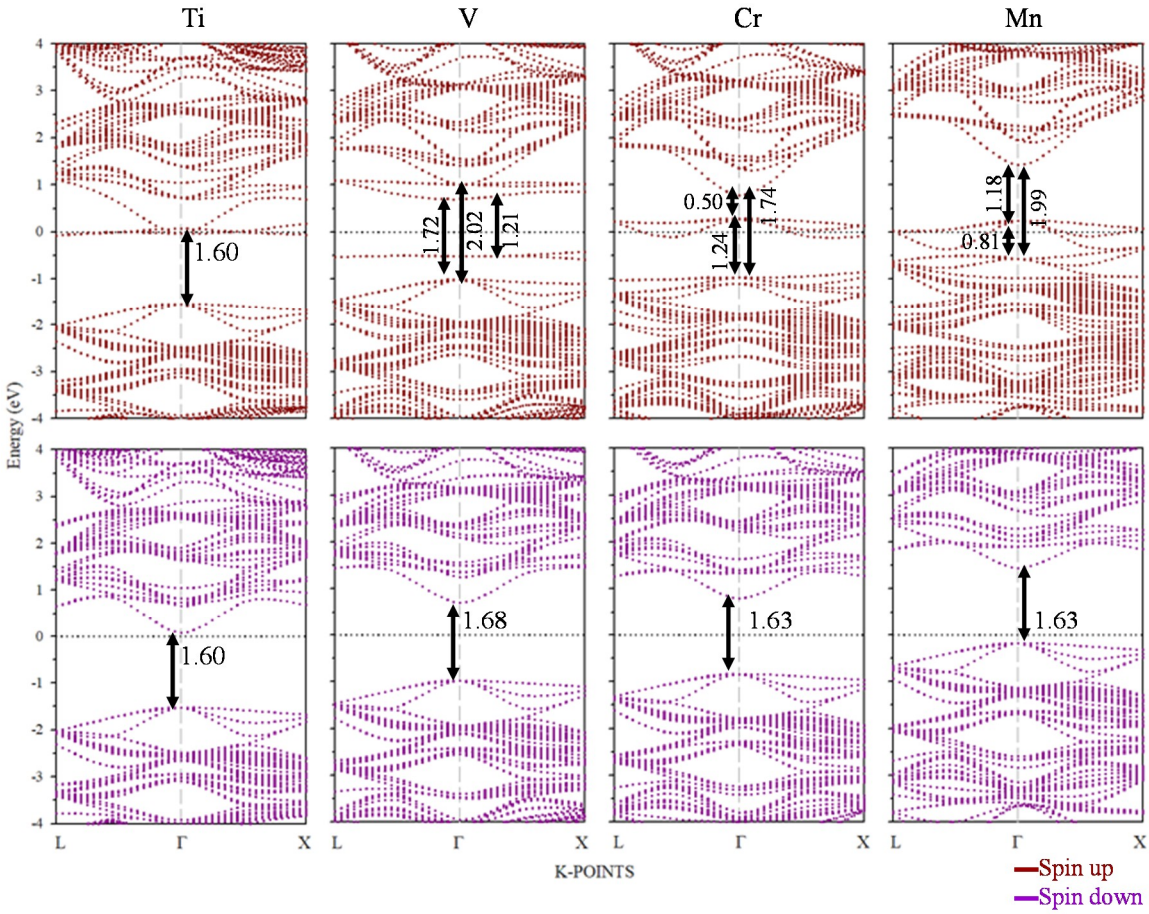

Figure S3. Electronic band structure of TM@InP (TM = Ti, V, Cr, Mn) calculated within G_0W_0 approach along to main energy differences at Γ-point. The zero of energy has been set at the Fermi level (black dotted line).

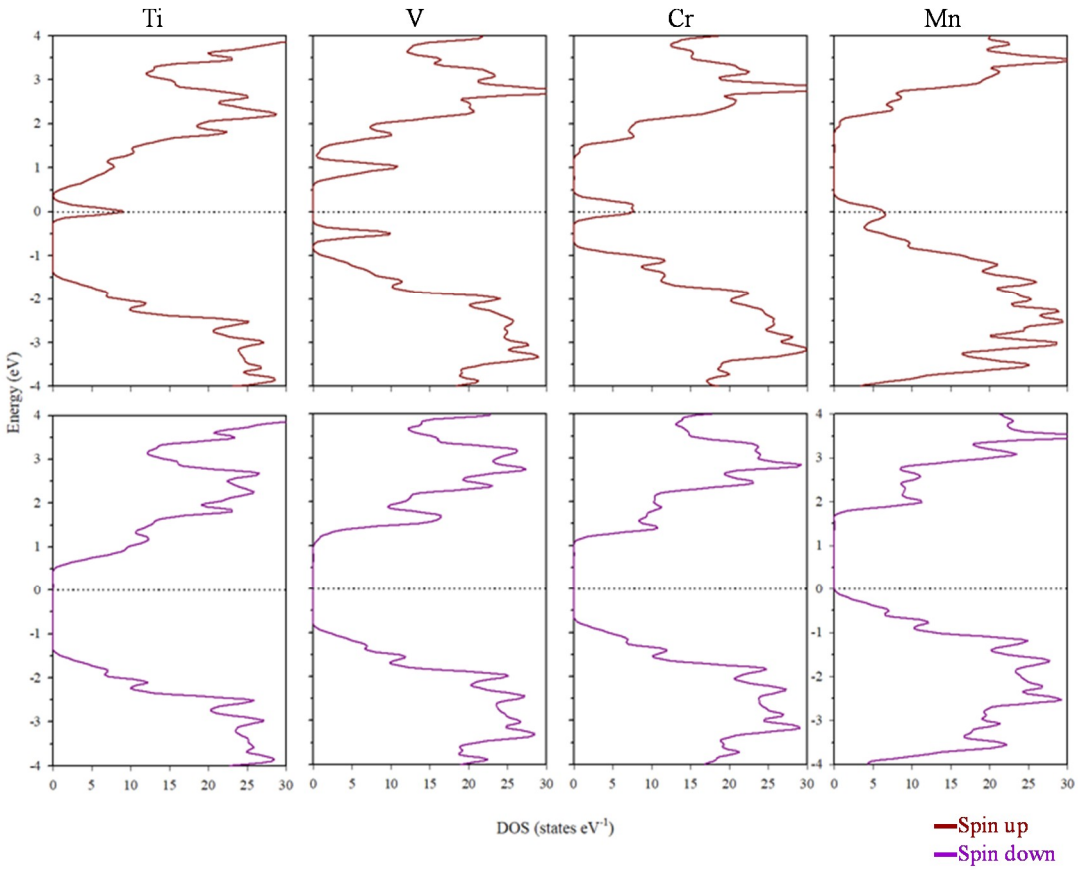

Figure S4. Density of States of TM@InP (TM = Ti, V, Cr, Mn) calculated within G_0W_0 approach. The zero of energy has been set at the Fermi level (black dotted line).