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### **Tailoring Ferromagnetic Semiconductors<sup>1</sup>**

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If magnetic semiconductors are ever to find wide application in real spintronic devices, their magnetic and electronic properties will require tailoring in much the same way that band gaps are engineered in conventional semiconductors. Unfortunately, no systematic understanding yet exists of how, or even whether, properties such as Curie temperatures and band gaps are related in magnetic semiconductors. We have explored theoretically these and other relationships within 64 members of a single materials class, the Mn-doped II-IV-V<sub>2</sub> chalcopyrites, three of which are already known experimentally to be ferromagnetic semiconductors. Our first-principles results reveal a variation of magnetic properties across different materials that cannot be explained by either of the two dominant models of ferromagnetism in semiconductors. Based on our results for structural, electronic, and magnetic properties, we identify a small number of new chalcopyrites with excellent prospects for stable ferromagnetism.

<sup>1</sup>In collaboration with Igor Zutic