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REPORT OF SCIENTIFIC STAY

My scientific stay took place at the institute of theoretical physics of the Technical University of Clausthal (Germany) within the group of Prof. Dr. Peter E. Blöchl.
We have started a new work on 3d-transition metal pyrite compounds, in the same spirit as our recently published one. The present investigation deals with the structural, electronic and magnetic properties of phosphorus substituting sulfur in iron disulfide i.e, $FeS_{2-x}P_x$, with different amounts $x = 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ and 1.

The calculations have been carried out using the CP-PAW code for ab-initio molecular dynamics and electronic structure calculations, which is the original implementation of the Projector Augmented Wave (PAW) method.
The main goal of the study is still looking for half metals. Here, however, this is carried out through light elements replacment (phosphorus replacing sulfur). First, we are considering only ferromagnetic alloys. where the calculations predict promising candidates for half metals.
Using GGA, a half-metallic behavior i.e, a full 100 % spin polarization has been obtained in the entire range of substitution ($x = 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ and 1). In such situation, we expect these materials to be of interest for spintronic applications, mainly as source for spin injection. Changing the density functional to hybrid functionals, the compounds tend to be ferromagnetic semiconductors. In the dilute limit ($x < \frac{1}{4}$), the material still could be intersting to use in spintronic, if it's Curie temperature is found to be near room one.

Our results are already written as a paper which is still in the initail stage of discussion and explanation. As in our previous work, we expect our results to have good impact in fondamental as well as applied research.

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