

**Project Title:**

**Magnetic properties of Gd/Co alloys**

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1. Background and purpose of the project, relationship of the project with other projects

Much effort has been devoted extensively in the research field of spintronics to create a new concept and functionality which can be utilized to develop the next generation spin-driven devices. Here a search of (ferro)magnetic materials is crucial. One stream of this line is of course in dilute magnetic semiconductors where magnetic impurities are introduced in otherwise non magnetic semiconductors (insulators). There, various interesting properties have been already reported including even a possible room temperature ferromagnet. This project is to search for a new ferromagnetic materials.

2. Specific usage status of the system and calculation method

Using first principles calculations based on density functional theory, electronic structures are calculated.

3. Result

Our systematic calculations found that 1) stoichiometric surfaces are non magnetic, 2) Hf rich non-stoichiometric surfaces are usually non magnetic, and 3) O rich non-stoichiometric surfaces are ferromagnetic and half metallic when surface reconstruction of oxygen bonding does not take place. The ferromagnetic surface state found here is mostly due to spin polarization of O 2p valence electrons at the surface layer, and is argued to be a novel pathway to ferromagnet for materials without magnetic ions. We have also calculated surface energy for all surfaces studied and discussed a possible reason for recent controversial observations of ferromagnetism in HfO<sub>2</sub>

4. Conclusion

We have proposed a new class of ferromagnet which can appear at surfaces of non magnetic materials

5. Schedule and prospect for the future

We would like to extend our study to interface and alloy systems.

6. If you wish to extend your account, provide usage situation (how far you have achieved, what calculation you have completed and what is yet to be done) and what you will do specifically in the next usage term.

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7. If you have a "General User" account and could not complete your allocated computation time, specify the reason.

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8. If no research achievement was made, specify the reason.

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**Fiscal Year 2009 List of Publications Resulting from the Use of RICC**

We are writing a paper right now.

**[Publication]**

We are writing a paper right now.

**[Proceedings, etc.]**

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