

Title: Strength of effective Coulomb interaction in two-dimensional 3d transition-metal halides and dichalcogenides: intrinsic ferromagnetic materials and Mott insulator

Name: Hanif Hadipour
Department of Physics, University of Guilan,
41335-1914, Rasht, Iran

Over the past years, several works have been performed focusing on various characteristics of two-dimensional (2D) materials. In the 2D compounds, synthesis of the 3*d* transition metal dichalcogenides (TMDCs) and transition metal halides (TM-halides) such as VSe_2, CrI3, etc has led to a huge experimental and theoretical interest due to the existence of incredibly rich correlated phenomena ranging from room temperature intrinsic ferromagnetism to charge density wave ordering, valley polarization, Mott phase, etc [1-3]. However, for most of them, the origin of the intrinsic ferromagnetism remained controversial and existence of strongly correlated phase is still in doubt. In this way, some other opposite studies indicate that for example the ferromagnetism seen in these materials is extrinsic 2D magnetism stemming from vacancies, or proximity effects which are not able to be precisely eliminated in 2D crystal growth.

To overcome these contradictory results that are related to magnetism and Mott behavior, we have determined directly the Coulomb matrix elements between correlated electrons and subsequently correlation strength *U/W* for all TMDCs and TM-halides in two common structures, namely octahedral 1*T* and trigonal 2*H* structures performing systematic *ab initio* calculation based on the constrained random-phase approximation (cRPA). Based on calculated *U* and exchange interaction *J* values, we discuss the tendency of the electron spins to order ferromagnetically. In the particular cases, our results indicate that experimentally observed MnX_2 (*X*=S, Se) and V*X*2 (*X*=S, Se) have an intrinsic ferromagnetic behavior in pristine form. Among the TM halides in the, the correlation strength *U/W* reaches a maximum in Ni*X*2 and Cr*X*3 (*X*=I, Br, Cl) with values much larger than the corresponding values in elementary TMs and other TM compounds.

The Coulomb parameters obtained from *ab initio* calculations not only provide a fundamental understanding of the correlated phenomena in TMDCs and TM-halides, but also these effective interactions can also be used in model Hamiltonians thus increasing the predictive power of model calculations.

Biography

Hanif Hadipour
Date of birth: 1982/3/20, Rasht, Iran
Married - A child
Assistant Prof. Physics Department & Guilan University, Rasht, Iran
Email:hanif_hadipour@guilan.ac.ir, hanifhadipour@gmail.com

Language:
Persian (native)
English

Education background:
Ph.D. September 2006 to September 2010
Physics Department, Sharif University of Technology, Tehran, Iran
Research position for 6 month at university of Vienna in the department of materials and physics under Professor Kresse guidance.

Publication in physical review:
1. E. Sasiuglu, H. Hadipour, C. Friedrich, S. Blugel, and I. Mertig, "Strength of effective Coulomb interactions and origin of ferromagnetism in hydrogenated graphene", Phys. Rev. B 95, 060408(R) (2017).
2. H. Hadipour, E. Şaşıoğlu, F. Bagherpour, C. Friedrich, S. Blügel, and I. Mertig, "Screening of long-range Coulomb interaction in graphene nanoribbons: Armchair versus zigzag edges", Phys. Rev. B 98, 205123 (2018).
3. H Hadipour, "Screening of Coulomb interaction and π magnetism in defected graphene", Phys. Rev. B 99, 075102 (2019).
4. A. Neroni, E. Sasiuglu, H. Hadipour, C. Friedrich, S. Blugel, I. Mertig, and M. Lezaic, "First-principles calculation of the effective on-site Coulomb interaction parameters for
Sr2ABO6 (A=Cr, Mn, Fe, Co, Ni, and B=Mo, W) double perovskites", Phys. Rev. B 100, 115113 (2019) .
5. H Hadipour and Y. Yekta, "Ab initio study of the effective Coulomb interactions and Stoner ferromagnetism in M2C and M2CO2 (M=Sc, Ti, V, Cr, Fe, Zr, Nb, Mo, Hf, and Ta)
MXenes" Phys. Rev. B 100, 195118 (2019).
6. A. Montaghemi, H. Hadipour, F. Bagherpour, A. Yazdani, and S. Mahdavifar, "Nonconventional screening of Coulomb interaction in hexagonal boron nitride nanoribbons" Phys. Rev. B 101, 075427 (2020).
7. Y. Yekta, H. Hadipour, E. Sasiuglu, C. Friedrich, S. Blugel, and I. Mertig "Effect of spin polarization on the screening of the Coulomb interaction in two-dimensional transition-metal Halides MX2 and MX3 (M=Ti,V,Cr,Mn,Fe,Co,Ni; X=Cl, Br, I), Phys. Rev. Materials 5, 034001 (2021).
8. Ab initio calculation of the effective Coulomb interactions in MX2 (M=Ti, V, Cr, Mn,
Fe, Co, Ni; X=S, Se, Te): intrinsic magnetic ordering and Mott phase, recently accepted in Phys. Rev. B (2022).

References

[1] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, D. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, W. Yao, Di Xiao, P. Jarillo-Herrero, and X. Xu,
Nature (London) 546, 270 (2017).
[2] K. L. Seyler, D. Zhong, D. R. Klein, Sh. Gao, X. Zhang, B. Huang, E. Navarro-Moratalla, L. Yang, D. H. Cobden, M. A. McGuire, W. Yao, D. Xiao, P. Jarillo-Herrero, and X. Xu, Nat. Phys. 14, 277 (2018).
[3] M. Bonilla, S. Kolekar, Y. Ma, H. C. Diaz, V. Kalappattil, R. Das, T. Eggers, H. R. Gutierrez, M. H. Phan, and M. Batzill, Nat. Nanotechnol. 13, 289 (2018).

Presenting author details

Full name: Hanif Hadipour
Personal email id: hanifhadipour@gmail.com
Mobile Number: 098-09111492748
Telephone Number: 098-013-33778635
Twitter account:
Linked In account: https://scholar.google.com/citations?user=gGSK-LoAAAAJ&hl=en
Session name/ number:
Category: (Oral presentation/ Poster presentation) both, the Oral is my first choice