

Electronic Structure of Graphene on Co₂FeSi Heusler Alloy

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Abstract. Due to high carrier mobility and long spin diffusion length graphene is a promising material for spintronics applications. In order to achieve effective spin transport and increase spin injection efficiency, graphene interfaces with highly spin-polarised materials, such as Heusler alloys, are needed. In this work, first-principles calculations of graphene/Co₂FeSi electronic structure are done in the frame of density functional theory. It is shown that the high percent of spin polarization in this system is combined with the linear dispersion of the π -states of graphene. The results suggest that the Co₂FeSi Heusler alloy is a promising candidate for graphene-based spintronic devices.

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REFERENCES

- [1] W. Han, R. Kawakami, M. Gmitra, J. Fabian, Graphene spintronics, *Nature Nanotechnology*, 2014, vol. 9, pp. 794–807.
- [2] S. Li, K.V. Larionov, Z.I. Popov, T. Watanabe, K. Amemiya, S. Entani, P.V. Avramov, Y. Sakuraba, H. Naramoto, P.B. Sorokin, S. Sakai, Graphene/Half-Metallic Heusler Alloy: A Novel Heterostructure toward High-Performance Graphene Spintronic Devices, *Advanced Materials*, 2020, vol. 32, no. 6, art. no. 1905734.
- [3] G.F. Li, Y. Du, T. You, Y. Tan, G.Q. Li, Y. Zhang, S. Liu, S. Epitaxy of half-metallic Heusler alloy Co_2MnSi on Ge(111) substrate via a graphene interlayer with $L2_1$ -ordered Co_2MnSi , *Applied Physics Letters*, 2022, vol. 120, no. 16, art. no. 162403.
- [4] G.F. Li, J. Hu, H. Lv, Z. Cui, X. Hou, S. Liu, Y. Du, Effect of graphene tunnel barrier on Schottky barrier height of Heusler alloy $\text{Co}_2\text{MnSi}/\text{graphene}/\text{n-Ge}$ junction, *Chinese Physics B*, 2016, vol. 25, no. 2, art. no. 027304.
- [5] D. Du, T. Jung, S. Manzo, Z. LaDuca, X. Zheng, K. Su, V. Saraswat, J. McChesney, M.S. Arnold, J.K. Kawasaki, Controlling the balance between remote, pinhole, and van der Waals epitaxy of Heusler films on graphene/sapphire, *Nano Letters*, 2022, vol. 22, no. 21, pp. 8647–8653.
- [6] G. Grebenyuk, S.M. Dunaevsky, E.Yu. Lobanova, D.A. Smirnov, I.I. Pronin, Formation of graphene-capped cobalt silicides, *Applied Surface Science*, 2019, vol. 470, pp. 840–845.
- [7] M.V. Gomoyunova, G.S. Grebenyuk, V.Yu. Davydov, I.A. Ermakov, I.A. Eliseyev, A.A. Lebedev, S.P. Lebedev, E.Yu. Lobanova, A.N. Smirnov, D.A. Smirnov, I.I. Pronin, Intercalation of Iron Atoms under Graphene Formed on Silicon Carbide, *Physics of the Solid State*, 2018, vol. 60, no. 7, pp. 1439–1446.
- [8] P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M.B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, Advanced capabilities for materials modelling with Quantum ESPRESSO, *Journal of Physics: Condensed Matter*, 2017, vol. 29, no. 46, art. no. 465901.
- [9] D. Vanderbilt, Soft self-consistent pseudopotentials in a generalized eigenvalue formalism, *Physical Review B*, 1990, vol. 41, no. 11, pp. 7892–7895.
- [10] P.E. Blöchl, Generalized separable potentials for electronic-structure calculations, *Physical Review B*, 1990, vol. 41, no. 8, pp. 5414–5416.
- [11] J.P. Perdew, J. Chevary, S. Vosko, K.A. Jackson, M.R. Pederson, D. Singh, Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation, *Physical Review B*, 1992, vol. 46, no. 11, p. 6671–6687.
- [12] H.J. Monkhorst, J.D. Pack, Special points for Brillouin-zone integrations, *Physical Review B*, 1976, vol. 13, no. 12, pp. 5188–5192.
- [13] S. Grimme, Semiempirical GGA-type density functional constructed with a long-range dispersion correction, *Journal of Computational Chemistry*, 2006, vol. 27, no. 15, pp. 1787–1799.
- [14] S. Wurmehl, G.H. Fecher, H.C. Kandpal, V. Ksenofontov, C. Felser, H.J. Lin, Investigation of Co_2FeSi : The Heusler compound with highest Curie temperature and magnetic moment, *Applied Physics Letters*, 2006, vol. 88, no. 3, art. no. 032503.
- [15] H. Mori, Y. Odahara, D. Shigyo, T. Yoshitake, E. Miyoshi, Electronic band structure calculations on thin films of the $L2_1$ full Heusler alloys $X_2\text{YSi}$ (X , Y = Mn, Fe, and Co): Toward spintronic materials, *Thin Solid Films*, 2012, vol. 520, no. 15, pp. 4979–4983.
- [16] J. Wintterlin, M.L. Bocquet, Graphene on metal surfaces, *Surface Science*, 2009, vol. 603, no. 10–12, pp. 1841–1852.
- [17] S.M. Dunaevskii, E.Yu. Lobanova, E.K. Mikhailenko, I.I. Pronin, Electronic Structure of Graphene on Silicon Carbide Intercalated with Silicon and Cobalt Atoms, *Physics of the Solid State*, 2021, vol. 63, no. 6, pp. 819–824.