VASPBANDUNFOLDING PUBLICATIONS

49 papers published up until **29**th **Sept, 2024**.

- [1] Chen, Junjie; Ma, Xingyu; Gong, Li; Zhou, Conghua; Chen, Jianlin; Lu, Yangfan; Zhou, Maojun; He, Haiping and Ye, Zhizhen, "Improving the performance of lead-free Cs₂AgBiBr₆ double perovskite solar cells by passivating Br vacancies,"
 - J. Mater. Chem. C, vol. 12, no. 35, pp. 14 074-14 084, 2024.
- [2] Chen, Nian Ke; Gao, Yu Chen; Zhao, Ji Hong; Li, Chun Hao; Chen, Qi Dai; Sun, Hong Bo; Zhang, Shengbai and Li, Xian Bin, "Inert Gas Element as Active Infrared-Absorption Source and Donor in Silicon for Forbidden-Wavelength Sensing,"
 - Adv. Opt. Mater., vol. 12, no. 20, 2024.
- [3] Cholsuk, Chanaprom; Çakan, Aslı; Suwanna, Sujin and Vogl, Tobias, "Identifying Electronic Transitions of Defects in Hexagonal Boron Nitride for Quantum Memories,"

 Adv. Opt. Mater., vol. 12, no. 13, p. 2 302 760, May 2024.
- [4] Ding, Pengfei; Lin, Jun Fa; Sun, Peihan; Lou, Rui; Fedorov, Alexander; He, Zhi Xiao; Ma, Huan; Zhou, Zuoping; Büchner, Bernd; Chen, Xi; Liu, Kai; Xia, Tian Long and Wang, Shancai, "Emergence of monolayer electron behavior in bulk van der Waals superlattice," *Phys. Rev. B*, vol. 109, no. 15, p. 155 115, Apr. 2024.
- [5] Gengor, G.; Celebi, O. K.; Mohammed, A. S.K. and Sehitoglu, H., "Continuum strain of point defects," *J. Mech. Phys. Solids*, vol. 188, p. 105 653, Jul. 2024.
- [6] Jiang, Xuance; Yilmaz, Turgut; Vescovo, Elio and Lu, Deyu, "Manipulating topological properties in Bi₂Se₃/BiSe/transition metal dichalcogenide heterostructures with interface charge transfer," *Phys. Rev. B*, vol. 109, no. 11, p. 115 112, Mar. 2024.
- [7] Meng, Qian; Bank, Seth R. and Wistey, Mark A., "Undoing band anticrossing in highly mismatched alloys by atom arrangement,"

 J. Appl. Phys., vol. 135, no. 11, p. 113 101, Mar. 2024.
- [8] Morris, Ian M.; Klink, Kai; Singh, Jaideep T.; Mendoza-Cortes, Jose L.; Nicley, Shannon S. and Becker, Jonas N., "Rare isotope-containing diamond colour centres for fundamental symmetry tests," *Philos. Trans. R. Soc. A Math. Phys. Eng. Sci.*, vol. 382, no. 2265, p. 20230169, Jan. 2024. arXiv: 2305.05781.
- [9] Novotny, Michal; Tkacova, Karolina and Karlicky, Frantisek, "The effect of mixed termination composition in Sc, Ti, and V-based MXenes," *Phys. Chem. Phys.*, 2024.
- [10] Sousa, Frederico B.; Zheng, Boyang; Liu, Mingzu; Resende, Geovani C.; Zhou, Da; Pimenta, Marcos A.; Terrones, Mauricio; Crespi, Vincent H. and Malard, Leandro M., "Effects of Vanadium Doping on the Optical Response and Electronic Structure of WS2 Monolayers,"

 Adv. Opt. Mater., vol. 12, no. 19, p. 2400 235, Jul. 2024.
- [11] Thomas, John C.; Chen, Wei; Xiong, Yihuang; Barker, Bradford A.; Zhou, Junze; Chen, Weiru; Rossi, Antonio; Kelly, Nolan; Yu, Zhuohang; Zhou, Da; Kumari, Shalini; Barnard, Edward S.; Robinson, Joshua A.; Terrones, Mauricio; Schwartzberg, Adam; Ogletree, D. Frank; Rotenberg, Eli; Noack, Marcus M.; Griffin, Sinéad; Raja, Archana; Strubbe, David A.; Rignanese, Gian Marco; Weber-Bargioni, Alexander and Hautier, Geoffroy, "A substitutional quantum defect in WS₂ discovered by high-throughput computational screening and fabricated by site-selective STM manipulation,"
 Nat. Commun., vol. 15, no. 1, p. 3556, Apr. 2024.
 - **Nat. Commun.**, vol. 15, no. 1, p. 3556, Apr. 2024. arXiv: 2309.08032.

arXiv: 2401.09402.

- [12] Ulstrup, Søren; in 't Veld, Yann; Miwa, Jill A.; Jones, Alfred J.H.; McCreary, Kathleen M.; Robinson, Jeremy T.; Jonker, Berend T.; Singh, Simranjeet; Koch, Roland J.; Rotenberg, Eli; Bostwick, Aaron; Jozwiak, Chris; Rösner, Malte and Katoch, Jyoti, "Observation of interlayer plasmon polaron in graphene/WS2 heterostructures," *Nat. Commun.*, vol. 15, no. 1, p. 3845, May 2024.
- [13] Woods, John M.; Chand, Saroj B.; Mejia, Enrique; Adhikari, Ashok; Taniguchi, Takashi; Watanabe, Kenji; Flick, Johannes and Grosso, Gabriele, "Emergent Optical Resonances in Atomically Phase-Patterned Semiconducting Monolayers of WS2."

- ACS Photonics, vol. 11, no. 9, pp. 3784-3793, Sep. 2024.
- [14] Xiong, Yihuang; Mathew, Milena; Griffin, Sinéad M.; Sipahigil, Alp and Hautier, Geoffroy, "Midgap state requirements for optically active quantum defects," Mater. Quantum Technol., vol. 4, no. 1, p. 013 001, Mar. 2024. arXiv: 2302.10767.
- [15] Xu, Jinhong; Zheng, Qijing and Zhao, Jin, "Spontaneous polarization dynamics in V-doped monolayer MoS₂," Comput. Mater. Today, vol. 1, p. 100 004, May 2024.

- [1] Cholsuk, Chanaprom; Suwanna, Sujin and Vogl, Tobias, "Comprehensive Scheme for Identifying Defects in Solid-State Quantum Systems,"
 - J. Phys. Chem. Lett., vol. 14, no. 29, pp. 6564–6571, Jul. 2023. arXiv: 2305.17889.
- [2] Kobayashi, Takuma; Shimura, Takayoshi and Watanabe, Heiji, "Oxygen-vacancy defect in 4H-SiC as a near-infrared emitter: An ab initio study," *J. Appl. Phys.*, vol. 134, no. 14, p. 145 701, Oct. 2023.
- [3] Kumar, Anand; Samaner, Çağlar; Cholsuk, Chanaprom; Matthes, Tjorben; Paçal, Serkan; Oyun, Yağız; Zand, Ashkan; Chapman, Robert J.; Saerens, Grégoire; Grange, Rachel; Suwanna, Sujin; Ateş, Serkan and Vogl, Tobias, "Polarization Dynamics of Solid-State Quantum Emitters," ACS Nano, vol. 18, no. 7, pp. 5270–5281, Feb. 2023. arXiv: 2303.04732.
- [4] Mohseni, Meysam; Udvarhelyi, Péter; Thiering, Gergo and Gali, Adam, "Positively charged carbon vacancy defect as a near-infrared emitter in 4H-SiC," *Phys. Rev. Mater.*, vol. 7, no. 9, p. 096 202, Sep. 2023. arXiv: 2305.17483.
- [5] Sánchez-Ramírez, Irián; Vergniory, Maia G.; Felser, Claudia and De Juan, Fernando, "Band structures of (NbSe4) 3 i and (TaSe4) 3 I: Reconciling transport, optics, and angle-resolved photoemission spectroscopy," Phys. Rev. B, vol. 107, no. 20, p. 205 109, May 2023.
- [6] Singha, Ratnadwip; Dalgaard, Kirstine J.; Marchenko, Dmitry; Krivenkov, Maxim; Rienks, Emile D.L.; Jovanovic, Milena; Teicher, Samuel M.L.; Hu, Jiayi; Salters, Tyger H.; Lin, Jingjing; Varykhalov, Andrei; Ong, N. Phuan and Schoop, Leslie M., "Colossal magnetoresistance in the multiple wave vector charge density wave regime of an antiferromagnetic Dirac semimetal,"

 Sci. Adv., vol. 9, no. 41, eadh0145, Oct. 2023.
- [7] Wildman, E. J.; Lawrence, G. B.; Walsh, A.; Morita, K.; Simpson, S.; Ritter, C.; Stenning, G. B.G.; Arevalo-Lopez, A. M. and Mclaughlin, A. C., "Observation of an exotic insulator to insulator transition upon electron doping the Mott insulator CeMnAsO,"

 Nat. Commun., vol. 14, no. 1, p. 7037, Nov. 2023.
- [8] Xiong, Yihuang; Bourgois, Céline; Sheremetyeva, Natalya; Chen, Wei; Dahliah, Diana; Song, Hanbin; Zheng, Jiongzhi; Griffin, Sinéad M.; Sipahigil, Alp and Hautier, Geoffroy, "High-throughput identification of spin-photon interfaces in silicon,"
 Sci. Adv., vol. 9, no. 40, eadh8617, Oct. 2023.
 arXiv: 2303.01594.

- [1] Agrawal, Sraddha; Vasenko, Andrey S.; Trivedi, Dhara J. and Prezhdo, Oleg V., "Charge carrier nonadiabatic dynamics in non-metal doped graphitic carbon nitride," *J. Chem. Phys.*, vol. 156, no. 9, p. 094 702, Mar. 2022.
- [2] Chen, Ping; Pan, Jinbo; Gao, Wenchao; Wan, Bensong; Kong, Xianghua; Cheng, Yang; Liu, Kaihui; Du, Shixuan; Ji, Wei; Pan, Caofeng and Wang, Zhong Lin, "Anisotropic Carrier Mobility from 2H WSe₂," *Adv. Mater.*, vol. 34, no. 7, p. 2 108 615, Feb. 2022.
- [3] Dardzinski, Derek; Yu, Maituo; Moayedpour, Saeed and Marom, Noa, "Best practices for first-principles simulations of epitaxial inorganic interfaces,"

 J. Phys. Condens. Matter, vol. 34, no. 23, p. 233 002, Jun. 2022.
- [4] Dhaliah, Diana; Xiong, Yihuang; Sipahigil, Alp; Griffin, Sinéad M. and Hautier, Geoffroy, "First-principles study of the T center in silicon,"

Phys. Rev. Mater., vol. 6, no. 5, p. L053201, May 2022. arXiv: 2202.04149.

- [5] Koch, Robert J.; Aryal, Niraj; Ivashko, Oleh; Liu, Yu; Abeykoon, Milinda; Bauer, Eric D.; Zimmermann, Martin V.; Yin, Weiguo; Petrovic, Cedomir and Bozin, Emil S., "Fluctuating Ru trimer precursor to a two-stage electronic transition in RuP,"
 - Phys. Rev. B, vol. 106, no. 21, p. 214516, Dec. 2022.
- [6] Krivenkov, M.; Marchenko, D.; Sajedi, M.; Fedorov, A.; Clark, O. J.; Sánchez-Barriga, J.; Rienks, E. D.L.; Rader, O. and Varykhalov, A., "On the problem of Dirac cones in fullerenes on gold," *Nanoscale*, vol. 14, no. 25, pp. 9124–9133, 2022.
- [7] Mayer, Justin A. and Seshadri, Ram, "Electron count dictates phase separation in Heusler alloys," *Phys. Rev. Mater.*, vol. 6, no. 5, p. 054 406, May 2022.
- [8] Newnham, Jon A.; Zhao, Tianqi; Gibson, Quinn D.; Manning, Troy D.; Zanella, Marco; Mariani, Elisabetta; Daniels, Luke M.; Alaria, Jonathan; Claridge, John B.; Corà, Furio and Rosseinsky, Matthew J., "Band Structure Engineering of Bi4O4SeCl2 for Thermoelectric Applications," ACS Org. Inorg. Au, vol. 2, no. 5, pp. 405–414, Oct. 2022.
- [9] Wang, Yongjie; Kavanagh, Seán R.; Burgués-Ceballos, Ignasi; Walsh, Aron; Scanlon, David and Konstantatos, Gerasimos, "Cation disorder engineering yields AgBiS₂ nanocrystals with enhanced optical absorption for efficient ultrathin solar cells,"

 Nat. Photonics, vol. 16, no. 3, pp. 235–241, Mar. 2022.
- [10] Yang, Shuyang; Schröter, Niels B.M.; Strocov, Vladimir N.; Schuwalow, Sergej; Rajpalk, Mohana; Ohtani, Keita; Krogstrup, Peter; Winkler, Georg W.; Gukelberger, Jan; Gresch, Dominik; Aeppli, Gabriel; Lutchyn, Roman M. and Marom, Noa, "Electronic Structure of InAs and InSb Surfaces: Density Functional Theory and Angle-Resolved Photoemission Spectroscopy,"

 Adv. Quantum Technol, vol. 5, pp. 3, p. 2100.033, Mar. 2022

Adv. Quantum Technol., vol. 5, no. 3, p. 2 100 033, Mar. 2022. arXiv: 2012.14935.

- [11] Yu, Jiawei; Xu, Zian; Xiao, Kebin; Yuan, Yonghao; Yin, Qiangwei; Hu, Zhiqiang; Gong, Chunsheng; Guo, Yunkai; Tu, Zhijun; Tang, Peizhe; Lei, Hechang; Xue, Qi Kun and Li, Wei, "Evolution of Electronic Structure in Pristine and Rb-Reconstructed Surfaces of Kagome Metal RbV3Sb5,"

 Nano Lett., vol. 22, no. 3, pp. 918–925, Feb. 2022.
- [12] Yuan, Shuaishuai and Bevan, Kirk H., "Engineering coexistence between free and trapped carriers via extrinsic polarons,"

 Phys. Rev. Mater., vol. 6, no. 11, p. 114 602, Nov. 2022.

- [1] Bae, Soungmin; Espinosa-García, William; Kang, Yoon Gu; Egawa, Noriyuki; Lee, Juho; Kuwahata, Kazuaki; Khazaei, Mohammad; Ohno, Kaoru; Kim, Yong Hoon; Han, Myung Joon; Hosono, Hideo; Dalpian, Gustavo M. and Raebiger, Hannes, "MXene Phase with C3 Structure Unit: A Family of 2D Electrides," *Adv. Funct. Mater.*, vol. 31, no. 24, 2021.
- [2] Davidsson, Joel; Ivády, Viktor; Armiento, Rickard and Abrikosov, Igor A., "ADAQ: Automatic workflows for magneto-optical properties of point defects in semiconductors," Comput. Phys. Commun., vol. 269, 2021. arXiv: 2008.12539.
- [3] Ding, Yiran; Zeng, Mengqi; Zheng, Qijing; Zhang, Jiaqian; Xu, Ding; Chen, Weiyin; Wang, Chenyang; Chen, Shulin; Xie, Yingying; Ding, Yu; Zheng, Shuting; Zhao, Jin; Gao, Peng and Fu, Lei, "Bidirectional and reversible tuning of the interlayer spacing of two-dimensional materials,"

 Nat. Commun., vol. 12, no. 1, p. 5886, Oct. 2021.
- [4] Gulyas, Istvan A.; Stephenson, Chad A.; Meng, Qian; Bank, Seth R. and Wistey, Mark A., "The carbon state in dilute germanium carbides,"

 J. Appl. Phys., vol. 129, no. 5, p. 055 701, Feb. 2021.
- [5] Krivenkov, M.; Marchenko, D.; Sánchez-Barriga, J.; Golias, E.; Rader, O. and Varykhalov, A., "Origin of the band gap in Bi-intercalated graphene on Ir(111)," 2D Mater., vol. 8, no. 3, p. 035 007, Jul. 2021.

[6] Lei, Shiming; Teicher, Samuel M.L.; Topp, Andreas; Cai, Kehan; Lin, Jingjing; Cheng, Guangming; Salters, Tyger H.; Rodolakis, Fanny; McChesney, Jessica L.; Lapidus, Saul; Yao, Nan; Krivenkov, Maxim; Marchenko, Dmitry; Varykhalov, Andrei; Ast, Christian R.; Car, Roberto; Cano, Jennifer; Vergniory, Maia G.; Ong, N. Phuan and Schoop, Leslie M., "Band Engineering of Dirac Semimetals Using Charge Density Waves," Adv. Mater., vol. 33, no. 30, p. 2 101 591, Jul. 2021. arXiv: 2009.00620.

[7] Liu, Zhonghao; Zhao, Ningning; Yin, Qiangwei; Gong, Chunsheng; Tu, Zhijun; Li, Man; Song, Wenhua; Liu, Zhengtai; Shen, Dawei; Huang, Yaobo; Liu, Kai; Lei, Hechang and Wang, Shancai, "Charge-Density-Wave-Induced Bands Renormalization and Energy Gaps in a Kagome Superconductor," Phys. Rev. X, vol. 11, no. 4, p. 041 010, Oct. 2021. arXiv: 2104.01125.

[8] Ortiz, Brenden R.; Teicher, Samuel M.L.; Kautzsch, Linus; Sarte, Paul M.; Ratcliff, Noah; Harter, John; Ruff, Jacob P.C.; Seshadri, Ram and Wilson, Stephen D., "Fermi Surface Mapping and the Nature of Charge-Density-Wave Order in the Kagome Superconductor CsV₃Sb₅," *Phys. Rev. X*, vol. 11, no. 4, p. 041 030, Nov. 2021. arXiv: 2104.07230.

[9] Qiu, Xiao Le; Gong, Ben Chao; Yang, Huan Cheng; Lu, Zhong Yi and Liu, Kai, "LaO as a candidate substrate for realizing superconductivity in an FeSe epitaxial film," *Phys. Rev. B*, vol. 103, no. 3, p. 035 143, Jan. 2021. arXiv: 2106.12388.

[10] Singha, Ratnadwip; Salters, Tyger H.; Teicher, Samuel M.L.; Lei, Shiming; Khoury, Jason F.; Ong, N. Phuan and Schoop, Leslie M., "Evolving Devil's Staircase Magnetization from Tunable Charge Density Waves in Nonsymmorphic Dirac Semimetals,"

Adv. Mater., vol. 33, no. 41, 2021. arXiv: 2107.06883.

- [11] Yuhara, Junji; Muto, Hiroaki; Araidai, Masaaki; Kobayashi, Masato; Ohta, Akio; Miyazaki, Seiichi; Takakura, Sho Ichi; Nakatake, Masashi and Lay, Guy Le, "Single germanene phase formed by segregation through Al(111) thin films on Ge(111),"

 2D Mater., vol. 8, no. 4, p. 045 039, Oct. 2021.
- [12] Zhang, Ruiqi; Lane, Christopher; Singh, Bahadur; Nokelainen, Johannes; Barbiellini, Bernardo; Markiewicz, Robert S.; Bansil, Arun and Sun, Jianwei, "Magnetic and f-electron effects in LaNiO2 and NdNiO2 nickelates with cuprate-like 3dx2-y2 band,"

 Commun. Phys., vol. 4, no. 1, p. 118, Jun. 2021.

____ 2020

[1] Davidsson, Joel, "Theoretical polarization of zero phonon lines in point defects," *J. Phys. Condens. Matter*, vol. 32, no. 38, p. 385 502, Sep. 2020. arXiv: 2002.11972.

[1] Vogl, Tobias; Sripathy, Kabilan; Sharma, Ankur; Reddy, Prithvi; Sullivan, James; Machacek, Joshua R.; Zhang, Linglong; Karouta, Fouad; Buchler, Ben C.; Doherty, Marcus W.; Lu, Yuerui and Lam, Ping Koy, "Radiation tolerance of two-dimensional material-based devices for space applications," *Nat. Commun.*, vol. 10, no. 1, p. 1202, Mar. 2019.

arXiv: 1811.10138.