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Editorial: Design of two-dimensional functional materials and nanodevices

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Editorial on the Research Topic
Design of two-dimensional functional materials and nanodevices

Two-dimensional (2D) materials and their heterostructures have attracted much attention in the fields of sensors, spintronic devices, thermoelectricity, battery, catalysis, photocatalysis, and optoelectronic devices due to their outstanding physical and chemical properties. In this Research Topic, entitled *Design of two-dimensional functional materials and nanodevices*, we collected a total of 17 articles reporting on the recent advances of 2D materials, heterostructures and materials with exotic topological and spintronic properties. Below, we provide a summary and research highlights on these exciting works.

Novel 2D sensing materials

Li et al. presented a recent research progress of gas sensing performance of 2D h-WO_3. The characteristics and the effects of microstructure, oxygen vacancy, and doping modification on the gas sensing performance of 2D h-WO_3 are summarized. The application of 2D h-WO_3 gas sensor and the challenges are discussed. Yong et al. investigated the N_2 and O_2 gas sensing properties of pristine and defective PtS_2 via first principles calculations, they found that the $PtSe_2$ with Pt@Se anti-site defect is a sensitive electrical and optical sensor for N_2 gas detection and the $PtSe_2$ with Pt vacancy, Se vacancy, Pt@Se anti-site defect are promising electrical and optical sensors for O_2 gas detection.

Novel 2D energy and environmental materials

Combining first-principles calculations and Boltzmann transport equations, Hu et al. explored the thermoelectric property of boron singlelayer. The boron layer possesses a low lattice thermal conductivity of 20.2 W/mK at 300 K. The boron singlelayer is a potential *p*-type thermoelectric material as its p-type the thermoelectric figure of merit is up to 0.96 at 300 K. By use of first principles calculations, Zhang et al. revealed the MoS_2-based Li- and Na-ions batteries show better cycle and rate performance than that of Mg- and Zn-ions batteries may be caused by the lower ions migration energy barrier, higher storage capability, and the phase transformation from 2H to 1T of Li- and Na-ions batteries. Sun used first principles calculations to explore the catalytic mechanism and activity of 11 types N-doped graphene. Among them, the zigzag pyridinic N- and zigzag graphitic N-doped graphene show excellent catalytic activity for CO_2 electrochemical reduction reaction in producing HCOOH.

Novel 2D van der waals heterostructures for photocatalytic water-splitting, optoelectronics and nanoelectronics

Combining different 2D materials to form van der Waals heterostructures (HS) provides a novel route to expand the application scope of 2D materials. Several HS with exceptional physical properties are predicted by first principles calculations. Ren et al. predicted that the CdO/As HS with a direct bandgap is a promising Z-type photocatalyst with the solar-to-hydrogen efficiency of 11.67%. Shao et al. found that $PtS_2/MoTe_2$ HS is a potential type-II photocatalyst for water-splitting with a novel light absorption, desirable band edge positions, and a proper potential drop. Shen et al. proposed that the lateral MoSSe/WSSe HS with type-II band alignment could be potentially applied in photocatalytic water-splitting. Besides, the heat flow transport is restricted by the natural bending caused by the asymmetric interface of the Janus MoSSe/WSSe HS. Ren et al. reported that AlN/Zr_2CO_2 HS with a type-I band alignment possesses potential application in light emitting devices. Xiao et al. effectively modulated the Schottky barrier height of graphene/ZnS HS by using horizontal and vertical strains.

Novel topological and spintronics materials

Yang et al. systematically evaluated the structural, magnetic, and electronic properties of Nd_2N and Nd_2NT_2 (T = OH, O, S, F, Cl, and Br), and the results showed that Nd_2NT_2 (T = OH, O, S, F, Cl, and Br) are all half-metals. Besides, the effects of strains and varied functional group proportions on their magnetic and electronic properties were also explored. Beyond 2D materials, this Research Topic also collects several articles reporting on the computational discovery of topological and other spintronic materials. Lin et al. proposed that pristine P63/mmc type TiTe is topological semimetal with type-I, type-II, and hybrid nodal lines. Chang et al. found that the hexagonal BaAgBi possesses two Weyl nodal ring states (or two Dirac nodal lines) with the absence (or presence) of spin–orbit coupling (SOC) effect. Zhang et al. reported that the NaCl with Fmm type structure possesses the triple point, quadratic contact triple point, linear and quadratic nodal lines in its phonon dispersion. Ding et al. developed the potential parameters for the Ti–Cr binary and the Ti–Cr–N ternary systems based on the second nearest-neighbor modified embedded-atom method. Hao et al. investigated the mechanical and thermodynamic effects caused by the interstitial and substitutional dopants of Ge, B, and He atoms to explore their effects on diamond wear. Dai et al. subtly modulated the growth temperature, duration time, and growth pressure to successfully achieve the controlled growth of γ-InSe and α-In_2Se_3 crystals with completely different stoichiometries and stacking manner of atomic layers.

We hope that this Research Topic can provide theoretical insights that are useful for the development and design of novel 2D functional material and heterostructure devices. We would like to thank all the authors, reviewers, and editors who contributed to the Research Topic.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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