Seminar: Hard Condensed Matter Theory

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Room: Galilei room, 01-128 (Staudingerweg 9**)**
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High throughput design of magnetic materials

Magnetic materials play an essential role in green energy applications as they provide efficient ways of harvesting/converting energies and engineering spintronic devices with low energy cost. The key questions nowadays are how to optimize the performance of existing systems and to design novel materials for broader applications. In this talk, our recent results on high throughput screening of functional magnetic materials will be presented. Using the in-house developed high throughput environment, the stabilities of antiperovskite, MAX, and quaternary Heusler compounds are investigated, resulting in many potential candidates for further experimental exploration. Particularly, we have identified all four types of spin gapless semiconductors in quaternary Heuslers, with interesting transport properties. Furthermore, in order to characterize the physical properties in a high throughput manner, we implemented a poor-man's algorithm to construct maximally localized Wannier functions. Based on the bulk-boundary correspondence, we successfully predicted 11 new 3D topological insulators and 4 2D topological materials. Using the Wannier functions, we also demonstrated that there exists strong piezospintronic effect in antiperovskite with noncollinear magnetic ground states.

All interested are cordially welcome!

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