凝聚态物理-北京大学论坛

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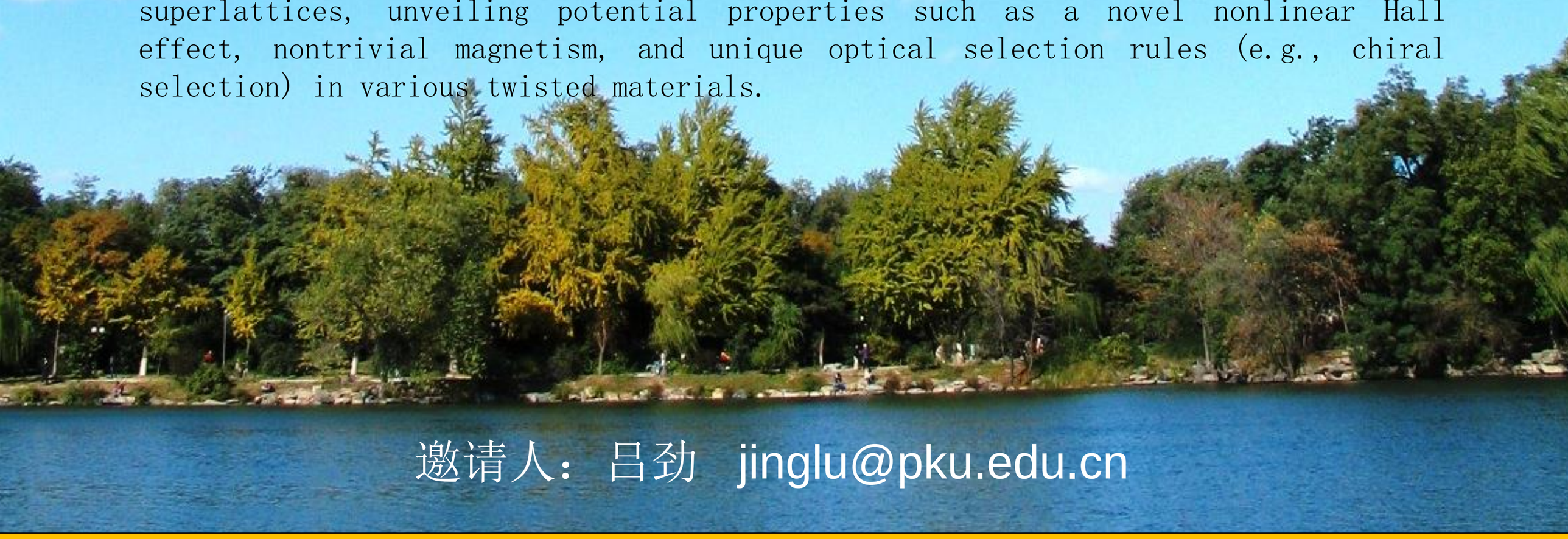
莫尔超晶格电子结构

宋志刚 研究员

时间：3月7日（星期四）15:00—16:30
地点：北京大学物理楼西563会议室

报告人简介（About speaker）：宋志刚，哈佛大学博士后。2012年本科毕业于郑州大学物理系，2017年获北京大学大学博士学位。2015-2016 年在麻省理工大学材料学院交流访问，导师李巨。2018-2021 美国加州大学伯克利分校和劳伦斯国家实验室开展博士后研究，导师汪林望。 2021年至今在美国哈佛大学开展博士后研究工作，导师Prineha Narang。至今，发表论文70余篇，被引用大约2800次（google scholar）。 以第一/共同第一/通讯作者身份在Science, JACS, Phys. Rev. Lett., Science advances, Advanced materials, Nano letters, ACS nano等期刊发表论文10余篇。2023 以重要作者获得美国能源部R&D 100 大奖。

摘要 (Abstract)：Current materials simulation faces computational limitations, prompting a keen interest in large-scale Density Functional Theory (DFT) algorithms. We have developed three distinct methods—ML-TB, charge density patching, and optimized atomic orbital DFT—each capable of computing the electronic structure of materials containing up to 100,000 atoms. Employing these advanced self-consistent calculations, we explored the electronic and optical properties of twisted bilayer systems and the possible applications in devices, without relying on any free parameters. Our investigations revealed artificial-atom states and quantum-dot arrays in twisted PbS, and we extended the computation of twistronics beyond van der Waals (vdW) materials, marking the first instance of a twisted structure non-vdW materials. Leveraging the localized and well-arranged states near the Fermi level in real space, we innovatively designed a new class of scalable qubits. Additionally, we delved into the geometry of 3D moiré superlattices, unveiling potential properties such as a novel nonlinear Hall effect, nontrivial magnetism, and unique optical selection rules (e.g., chiral selection) in various twisted materials.



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