北京大学量子材料科学中心

In e na onal Cen e fo Q an m Ma e ial PKU

Semina r

Fir -Principle Ma erial Theor , Di co er and De ign of Elec ronic and Op oelec ronic Ma erial

X a Q a

Depa men of Ma e ial Science and Enginee ing

Te a A&M Uni e i , USA

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V : R W563, P c b d , P U

地点：北京大学物理楼，西563会议室

Recen ad ance in fi -p inciple elec onic c e heo and high-pe fo mance high- h o ghp l comp ing ha e empo e ed effi ien comp a ion-aided di co e and de ign of no el ma e ial , pa ic la l impo an fo eme ging ene g and de ice echnologie . In hi alk, I ill highligh a fe e ample of o k on ma e ial di co e and de ice de ign enabled b fi -p inciple heo . Fi , I ill p e en heo e ical di co e and e pe imen al in e iga ion of 2D and 3D opological ma e ial incl ding Peie l -di o ed 1T and T_d bina and e na an i ion me al dichalcogenide (WTe_2, $MoTe_2$, $TaIrTe_4$, $TaRhTe_4$, $NbIrTe_4$, $NbRhTe_4$). We ill al o di c he elec ic field, ela ic ain, and an de Waal acking ind ced opological pha e an i ion and hei po en ial applica ion fo opo onic ch a opological field effec an i o . Second, I ill epo o ecen di co e of ongl co pled fe oelec ic-fe oela ic m l ife oic in 2D g o p IV monochalcogenide . The e 2D m l ife oic po e a fe di inc cha ac e i ic incl ding ongl -co pled gian fe oelec ici and fe oela ici , la ge ani o opic e ci onic op ical p ope ie i h i ible- pec m e ci onic gap and i able e ci on binding ene gie , and lo domain all ene g and mig a ion ba ie gge ing hei g ea po en ial fo nable m l ife oic f nc ional de ice b manip la ing e e nal elec ical, mechanical, and op ical field o con ol he in e nal ph ical e pon e , ch a 2D m l ife oic memo ie , fe oelec ic e ci onic pho o ol aic , and non ola ile m l ife oic pho onic memo . Finall , I ill p e en ome fi -p inciple me hodolog de elopmen o a d mo e acc a e and efficien p edic ion o e pedi e high- h o ghp ma e ial di co e and de ign fo no el ene g and de ice applica ion ..

D . Xiaofeng Qian i an a i an p ofe o in he Depa men of Ma e ial Science and Enginee ing a Te a A&M Uni e i , o king on fi -p inciple ma e ial heo , di co e , and de ign fo ene g and de ice applica ion . D . Qian ob ained hi bachelo deg ee in Enginee ing Ph ic f om T ingh a Uni e i in China in 2001, and ece i ed hi Ph.D. deg ee in N clea Science and Enginee ing f om Ma ach e In i e of Technolog in 2008. He hen o ked i h P of. Nicola Ma a i and P of. J Li a a po doc a MIT on he fi -p inciple e ci ed a e me hodolog and 2D ma e ial and de ice de ign, and joined Te a A&M Uni e i in 2015. Hi g o p i c en l foc ing on fi -p inciple heo of ligh - ma e in e ac ion a he nano cale.

冯济