Computational Design of New Energy Materials and its Challenges

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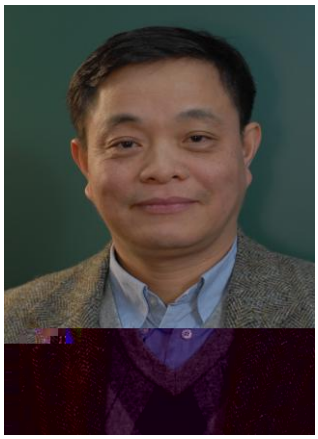
With the rapid development of the modern computational techniques, computational studies on the condensed matter, simulating specific dynamics processes and designing desired materials, have played a more and more important role. In this talk, I will take new solar energy materials, a quaternary semiconductor alloy we have worked on for a few years, as an example, to demonstrate the capability of computational designs of materials. I will show, by combining of some basic physical intuition, how we can clarify their structures and electronic properties of complicate quaternary alloys starting with well-known binary alloys, how we can extract the unique physics in such quaternary alloys which is absent in conventional semiconductors. Furthermore, I will present a new algorithm for inverse design with desired properties. Some of new elemental solar energy materials will be discussed. Finally, I will briefly discuss some key challenges in computational design of solar energy materials.



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