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PLENARY: Understanding and designing novel nanomaterials from first principles

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Abstract content
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Advances in theoretical methods for calculating the properties of materials from first principles, aided by the ever-continuing development of faster computers, now enable us to gain insight into why materials possess the properties they do. Such insights can then be leveraged so as to enable us to "rationally" design new materials that are tailored for specific applications.

After a brief general survey of recent advances in such methods, with special emphasis on ab initio density functional theory, I will cite some examples from work in my group. For example, in the field of nanoscale alloys, we have shown that Fe and Au, though bulk-immiscible, form a two-dimensional surface alloy that is stabilized by magnetic interactions; this prediction was confirmed by experiments in the group of Sylvie Rousset. Another prediction, that conceivably has applications for nanocatalysis, was our prediction that depositing gold nanoparticles on an oxide substrate that has been doped with an electron donor would change the morphology of the particles from three-dimensional to two-dimensional; this idea was subsequently shown to work by experiments in the group of Hajo Freund. We have also shown that there is reason to believe that the change in morphology is accompanied by an improvement in catalytic properties. We have also recently shown how the oxidation state of nanomaterials can be tuned by varying their size and environment; as a part of this study, we have suggested a novel yet simple way to interpret experimental data from XANES.

In the field of computational design of materials, one is increasingly placing greater emphasis on the development of 'descriptors', which can then be utilized to screen a large number of candidate materials quickly. I will describe some efforts in our group to develop such descriptors.

I will conclude my talk with some brief remarks about the relevance of carrying out programs of computational physics in a developing country, and the possibility of carrying out interesting research even with modest computational resources.

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