CELOÚSTAVNÍ SEMINÁŘ
Ústavu fyziky materiálů AV ČR

dne **27.5.2011** (pátek) v **11:00 h**
v přednáškovém sále (4. patro)
Ústavu fyziky materiálů AV ČR, Žižkova 22, Brno

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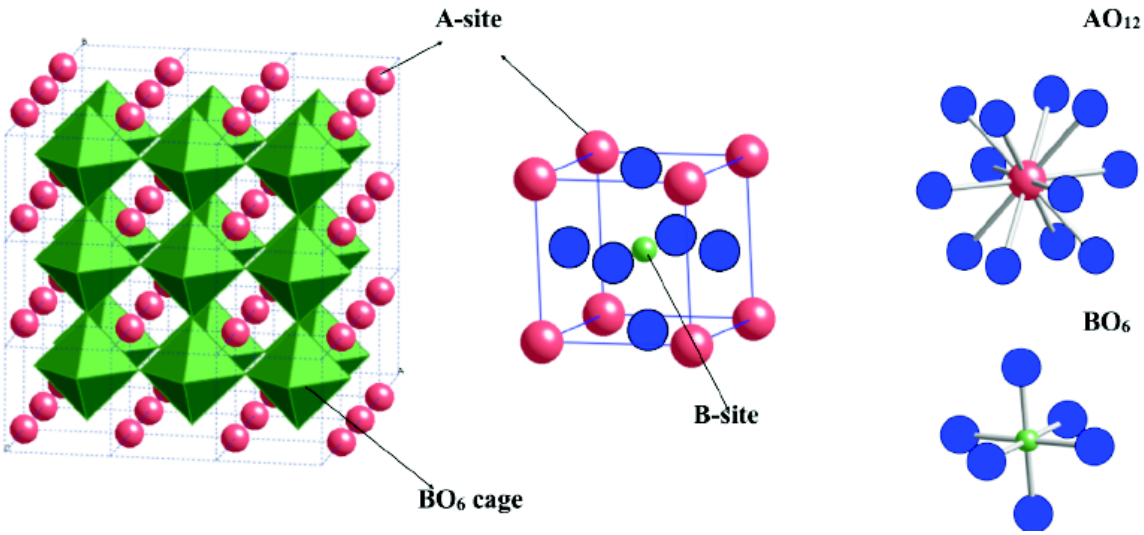
Statistical Learning for Materials Discovery and Design

Materials informatics permits one to survey complex, multiscale information in a high throughput, statistically robust and yet physically meaningful manner. The application of such approaches can have a significant impact in materials design and discovery. The mathematical and computational foundations of informatics lie in the fields of statistical learning and data mining. This presentation explore how the tools of statistical learning can be used to systematically integrate diverse attributes of chemical and electronic structure descriptors of atoms with descriptors associated with crystal structure of compounds to capture complexity in crystal geometry and bonding. Using informatics, we have been able to discover new compounds with targeted functionalities, the chemical design rules governing the stability of these compounds as well new structure-property relationships. It is shown that data mining methods can be extended far beyond just searching for information in databases and in fact serve as a robust tool for developing predictive physics based models.



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