
 **Computational  
Materials Physics** 

Center for  
Molecular  
Modeling

Department of  
Materials Science  
and Engineering

**“ab initio” :  
what does it mean ?**

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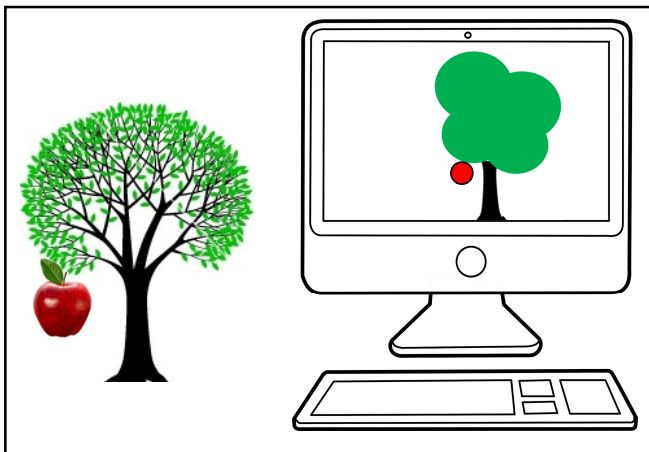
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recreate  
the observable facts of Nature  
in a  
mathematical model

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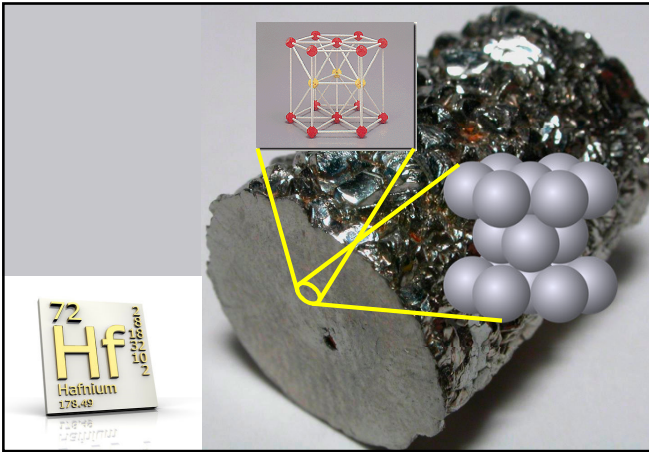
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recreate  
the observable facts of Nature  
in a  
mathematical model

$$\hat{H}\Psi = E\Psi \quad \rightarrow \quad V_{zz}$$

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