US-Africa Initiative Workshop

APS March Meeting - Sunday, March 14, 2021

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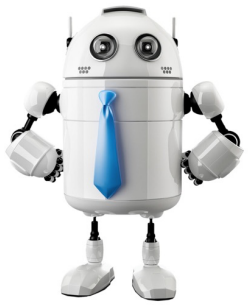
Software Advances for Mineral Physics Applications (SAMPA)



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I work in Prof. Renata Wentzcovitch's group. My research interests are using quantum mechanical theories and computational methods to investigate materials properties at planetary interior conditions and their geophysics implications. Density functional calculations, molecular dynamics, and lattice dynamics are some major approaches we used in our group.

My current colleagues collaborators include Jingyi Zhuang, Hongjin Wang, Yang Sun, etc. We have investigated the thermodynamic properties of ε-Fe with thermal electronic excitation effects on vibrational spectra, using an extended version of my code for quasi-harmonic approximation calculations. For now, I am developing software for workflows that not only reduce the human labor and computational cost in our daily work but also bind the programs we have developed under a unified interface. We also have other interesting projects hosted on our GitHub organization.

It would be great to collaborate on developing computational physics software or new algorithms and methods. I will also be glad to apply these codes/methods to study (planetary) materials at extreme conditions and explore intriguing geophysics topics.

My talk: Express: nonstop calculations with Quantum ESPRESSO
On 5:12 PM–5:24 PM, Wed, 17th March Session P19