PHYSICS COLLOQUIUM:
Doped two-dimensional materials: simulations of Raman spectroscopy, friction, and distorted phases

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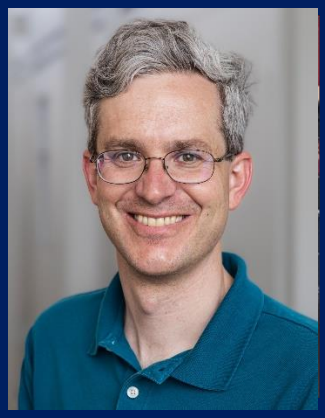
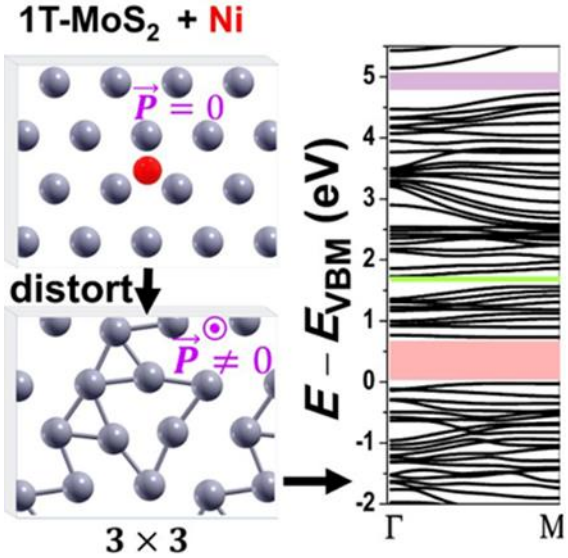


About The Speaker:

David Strubbe is an associate professor of physics and chair of the physics PhD program at the University of California, Merced. He was a postdoc in materials science and engineering at the Massachusetts Institute of Technology. He received his PhD in 2012 in the research group of Steven G. Louie at the Department of Physics, UC Berkeley, and was an NSF and Nano-IGERT fellow. He received a B.S. in chemistry and physics at the University of Chicago in 2005. He has received the NSF CAREER award and the Cottrell Scholar Award from the Research Corporation for Science Advancement.



Abstract:

Doping 2D materials can tune their electronic, optical, magnetic, catalytic, and mechanical properties, but it is difficult to get conclusive evidence from experiments about where the dopants are located, particularly in multilayer or bulk materials. Raman spectroscopy can be a powerful tool for characterization but help from simulations is needed to interpret the spectra in terms of dopant location in substitutional or intercalation sites. In Ni-doped MoS_2, important for catalysis and lubrication, we find distinct fingerprints of the different doping sites and analyze their origin. In Re-doped MoS_2, important for electronics, we again find distinct characteristics of the doping sites, mostly in terms of shifts of the pristine Raman peaks with a complex origin. In an experimental collaboration, we used these results to identify the location of dopants in samples of Re-doped MoS_2 that showed an unusual increase in nanoscale friction with the number of layers. We have extended these results also to examine new structural and electronic and multiferroic phases resulting from Ni-doping of 1T-MoS_2, investigate the mechanisms of sliding friction in Ni-doped MoS_2, and parametrize a ReaxFF classical force field for use in study of mechanical properties. Finally, I will show some results from an undergraduate/graduate class project in which students calculated Raman spectra of $MoS_{2x}Se_{2(1-x)}$ monolayer alloys.

Date:
1/19/2024

Time:
10:30 AM - 11:50 AM

Location:
GRANITE PASS 135

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