

Mechanisms for Surface-enhanced Raman Effect on 2D Materials: A First Principles Study**Speaker:** He Wen

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Date: 5th Sep 2019, Thursday
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Venue: EA-06-03

Abstract

Surface-enhanced Raman Spectroscopy (SERS), benefitting from enhancement of Raman signals of probe molecules in vicinity of a substrate, has translated into many applications to detect and analyze trace concentrations of molecules. Due to absence of the electromagnetic mechanism, 2D materials like graphene provide a platform for a fundamental study of the unconventional enhancement mechanism for SERS. Though recent studies have pointed to charge transfer and dipole-dipole interaction to be responsible for the enhancement mechanism, a clear understanding of the enhancement mechanism is still lacking. In this study, we perform first-principle calculations to explore the enhancement mechanism for SERS on 2D substrates. For this, we use the small organic molecule, pyridine, as a probe molecule and monolayer h-BN, SnS and BP as substrates. We focus on both the non-resonant and resonant Raman spectra polarized in-plane (XX and YY) and out-of-plane (ZZ), with respect to the substrate. For non-resonant Raman spectra, we find the dielectric constant of the substrate plays the significant role in the enhancement effect. In addition, weak van der Waals interactions between the molecule and the substrate induce Raman enhancement of some out-of-plane modes. The Raman enhancement effect in resonant Raman spectra at DFT level is in progress. And the study at GW level as well as including excitonic effects will be the major topic of further investigation to provide insights into the light-matter coupling in these organic-2D material heterostructures.

He Wen received her bachelor's degree in Department of Materials and Engineering from Harbin Institute of Technology. She is now a PhD candidate in Department of MSE under A/P Quek Su Ying and Prof. Pennycook, Stephen John. Her current research mainly focuses on the first principles calculations of Raman spectra.

ALL ARE WELCOME!

Host: A/P Xue Junmin