Probing the temperature evolution of experimentally forbidden E_{1g} (E") and A_{2u} (A"$_2$) modes in monolayer MoS_2 using classical molecular dynamics simulations

P. Anees[1], M.C. Valsakumar[2] and B. K. Panigrahi[3]

[1]Materials Physics Division, Indira Gandhi Centre for Atomic Research, Kalpakkam, 603 102, India

[2]Department of Physics, Indian Institute of Technology, Kozhippara, Palakkad, 678 557, India

anees@igcar.gov.in

Abstract

Temperature dependent frequency shift and linewidth of Γ point optic modes in monolayer MoS_2 are studied using classical molecular dynamics simulations. In this study, for the first time, we reports the temperature evolution of experimentally forbidden Raman active E_{1g} (E") and infra-red (IR) active A_{2u} (A"$_2$) modes, in-addition to the previously reported Raman active E_{2g} (E') and A_{1g} (A'$_1$) modes. All the modes are showing a redshift with temperature. We delineated the contribution of anharmonic coupling of phonon modes and thermal expansion to the total frequency shift and linewidth, and found that strong anharmonic coupling of phonon modes is the predominant source of observed redshift and broadening of peaks, the thermal expansion contribution is negligible. The temperature dependence of all modes is quantified by computing the first-order temperature co-efficient.