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Evolution of Raman active mode in linear acetylenic Carbon chains. ALDO RAELIARIJAONA, JORGE ALARCON OCHOA, HUMBERTO TERRONES, Rensselaer Polytechnic Institute, YUNG JOON JUNG, Northeastern University — We investigate the Raman signatures of linear Carbon chains using first-principles calculations, namely Density Functional Theory, Density Functional Perturbation Theory as well as molecular dynamics techniques. Our studies of the linear acetylenic Carbon chains (CnH2) of varying lengths (n=2 to n=60) focus on: a) the identification of the Longitudinal Optic (LO) mode by using its phonon eigenvector and eigenvalue for each Carbon chain length, b) tracking the evolution of the LO mode in question with respect to chain length. Our analyses reveal that: 1. the LO modes tend to soften with increasing chain length, 2. the vibration signal of unstrained acetylenic Carbon chain of length n=24 matches well that of the Coalescence Inducing Mode (1850 cm-1) of Carbon nanotubes, 3. short acetylenic chains may also be responsible for the CIM Raman signal but require tensile strain to soften their vibration further, 4. as the acetylenic Carbon chain grow longer, higher harmonics (2nd or 3rd) LO vibrations can be present and for longer chains these higher harmonics mode exhibit Raman signals close to the CIM value of 1850 cm-1.

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