Capacity Enhancement of Polylithiated Functionalized Boron Nitride Nanotubes: An Efficient Hydrogen Storage Medium

Puspamitra Panigrahi^{*1}, Ashok Kumar¹, Hyeonhu Bae², Hoonkyung Lee², Rajeev Ahuja^{3, 4} and Tanveer Hussain^{*5}

¹Centre for Clean Energy and Nano Convergence, Hindustan Institute of Technology and Science, Chennai 603103, Tamil Nadu, India.

²Department of Physics, Konkuk University, Seoul 05029, Republic of Korea

³Condensed Matter Theory Group, Department of Physics and Astronomy, Box 516,

Uppsala University, S-75120 Uppsala, Sweden

⁴Applied Materials Physics, Department of Materials and Engineering, Royal Institute of Technology (KTH), S-100 44 Stockholm, Sweden

⁵School of Molecular Sciences, The University of Western Australia, Perth, WA 6009, Australia

Corresponding author: tanveer.hussain@uwa.edu.au, akshaymitra@gmail.com



Fig. S1: Phonon vibration modes along different wave vectors along with gamma point.