Searching for higher superconducting transition temperature in strained MgB$_2$ using first principles calculations  

JIN-CHENG ZHENG, Brookhaven National Laboratory, YIMEI ZHU, Brookhaven National Laboratory — Since the discovery of the amazing high superconducting transition temperature ($T_c$) in non-oxide MgB$_2$, great efforts have been made on the search for higher $T_c$ in MgB$_2$ and related materials by either chemical substitutions or by applying pressures to modify the lattice of MgB$_2$. Little success has been achieved so far due to the fact that the $T_c$ is always suppressed using either method. To tailor the $T_c$ in MgB$_2$, the full atomic-level understanding of underlying mechanism of chemical and lattice effects is required. According to the McMillan-Allen-Dynes analysis, $T_c$ in MgB$_2$ is controlled by the collective contributions from phonon frequency, electron-phonon coupling and Coulomb repulsion. Consideration of one single parameter alone cannot guarantee the improvement of $T_c$ because of the strong coupling and competing of other parameters. Here we present a detailed first-principles density functional analysis of the effects of lattice strains to superconducting properties of MgB$_2$. On the basis of our results for structural, electronic, vibrational and superconducting properties of strained MgB$_2$, we show how higher superconducting transition temperature might be achieved in strained MgB$_2$ superconductor.