Supplementary Information (SI) for Physical Chemistry Chemical Physics.
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First-Principles Prediction of β-phase SnA_2N_4 (A = Si; Ge) Monolayers: Outstanding Mechanical Anisotropy and High Electron Mobility for FET Devices

Yi Peng [a] ; Minjia Yao[a]; Fangyuan Li [a]; Yu Chen [a]; Yana Li [a]; Shuangmei Qian [a];Qianqian Zhu*[a]; Juexian Cao*[b]

a: *Microelectronics and Optoelectronics Technology Key Laboratory of Hunan Higher Education, School of Physics and Electronic Electrical Engineering, Xiangnan University, Chenzhou 423000, P. R. China*

b: *Hunan Institute of Advanced Sensing and Information Technology, Xiangtan University, Xiangtan 411105, PR China*

* E-mail address: pengzhu2022@ yeah.net

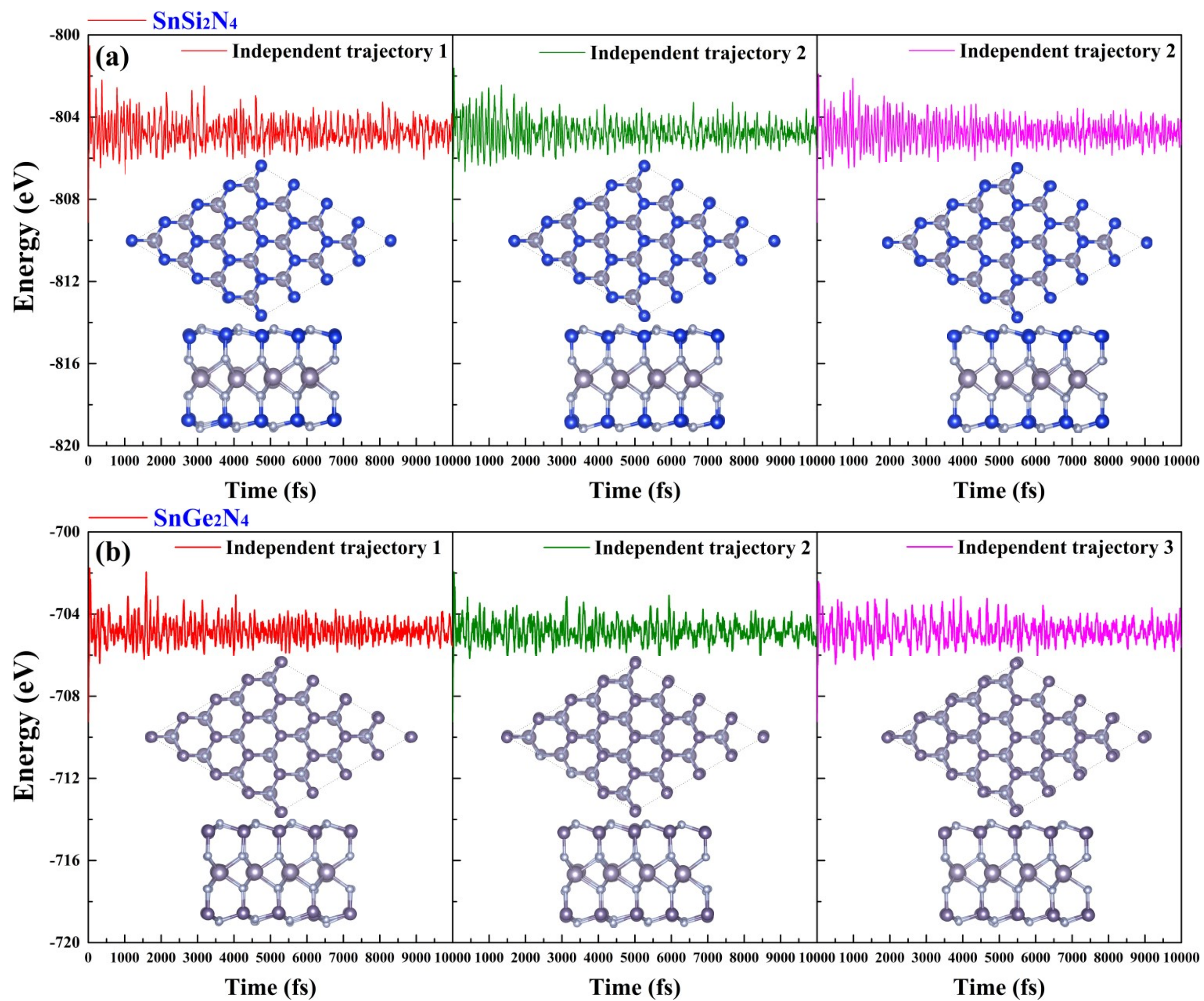

Fig. S1. Calculated AIMD simulations of (a) β-$SnSi_2N_4$ and (b) β-$SnGe_2N_4$ monolayers from three independent trajectories (10 ps, 300 K).

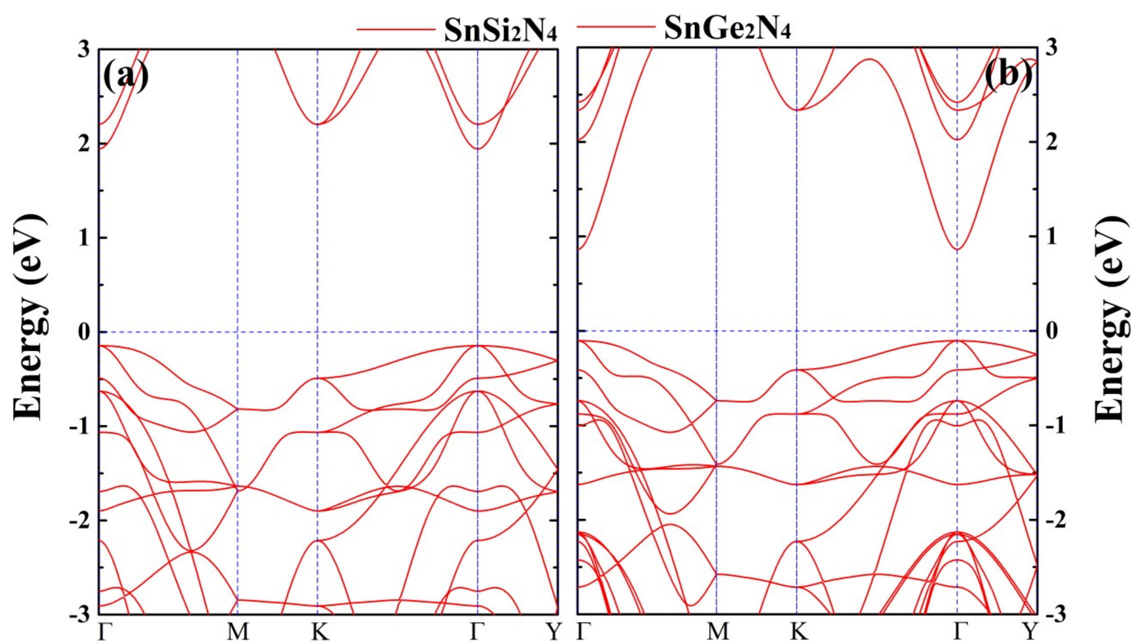

Fig. S2. Calculated band structure of orthogonal β-$SnSi_2N_4$ (a) and β-$SnGe_2N_4$ (b) monolayers

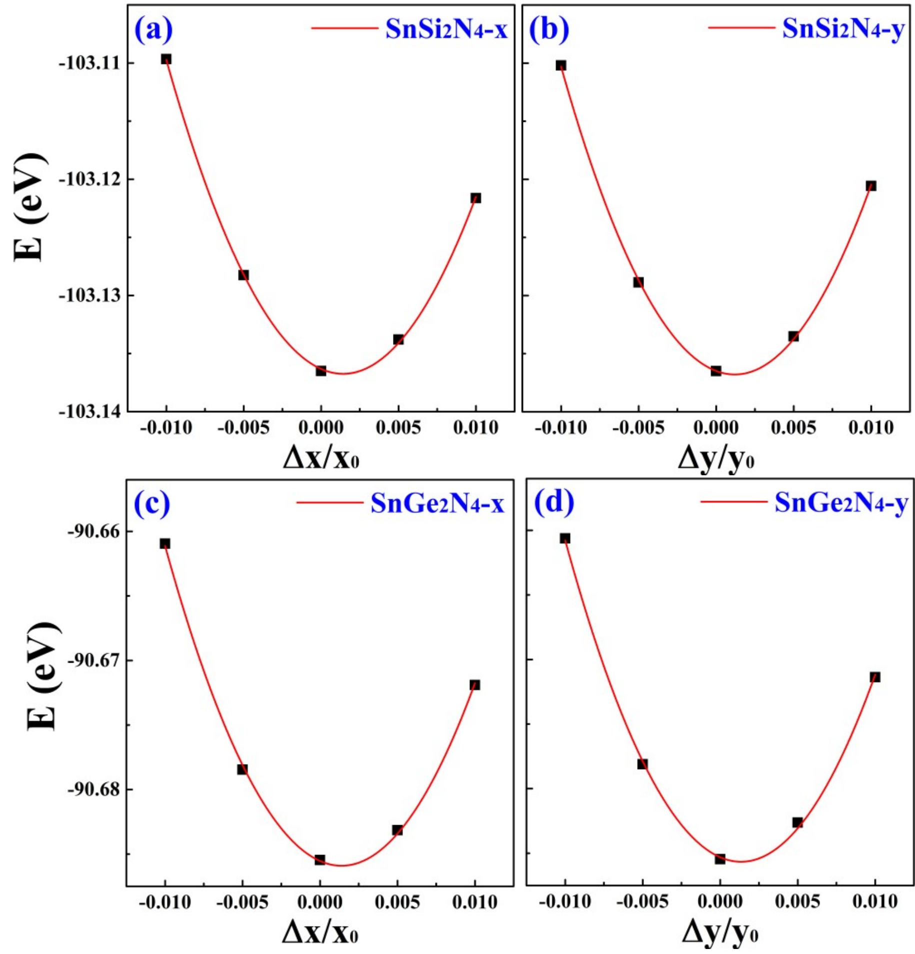

Fig. S3. Total energy of β-$SnSi_2N_4$ and β-$SnGe_2N_4$ monolayers as a function of uniaxial strain along the x and y directions, respectively. The in-plane stiffness *C* can be obtained after fitting the parabola.

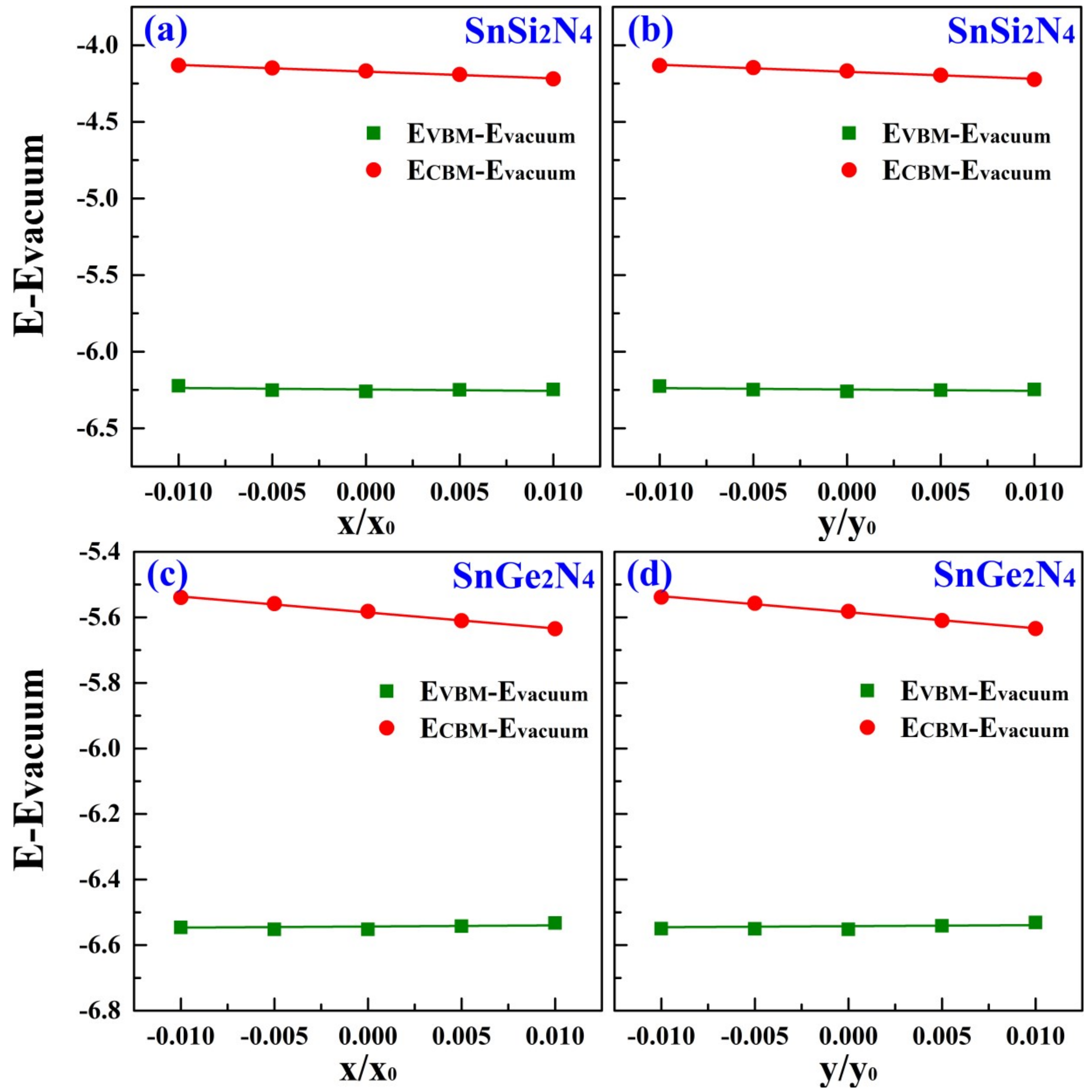

Fig. S4. Band edge positions (CBM and VBM) of β-$SnSi_2N_4$ and β-$SnGe_2N_4$ monolayers, referenced to the vacuum level, as a function of lattice strain along the x (a,c) and y (b,d) directions. The slopes of the linear fits to CBM (red circles) and VBM (green squares) correspond to the deformation potential constants for electrons and holes, respectively.