## Supplementary Information Novel two-dimensional of AISb and InSb monolayers with double-layer honeycomb structure: A Firstprinciple study

A. Bafekry<sup>1,2†</sup>, M. Faraji<sup>3</sup>, M. M. Fadlallah<sup>4</sup>, H. R. Jappor<sup>5</sup>, S. Karbasizadeh<sup>6</sup>, M. Ghergherehchi<sup>7,†</sup>, I. Abdolhosseini Sarsari<sup>6</sup>, A. Abdolahzadeh Ziabari<sup>8</sup>,

<sup>1</sup> Department of Radiation Application, Shahid Beheshti University, 19839 69411 Tehran, Iran. <sup>2</sup> Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium.

<sup>3</sup> TOBB University of Economics and Technology, Sogutozu Caddesi No 43 Sogutozu, 06560, Ankara, Turkey.

<sup>4</sup> Department of Physics, Faculty of Science, Benha University, 13518 Benha, Egypt.

<sup>5</sup> Department of Physics, College of Education for Pure Sciences, University of Babylon, Hilla, Iraq.

<sup>6</sup> Department of Physics, Isfahan University of Technology, Isfahan, 84156-83111, Iran. <sup>7</sup> Department of Electrical and Computer Engineering, Sungkyunkwan University, 16419 Suwon, Korea. Email: mitragh@skku.edu <sup>8</sup> Nano Research Lab, Lahijan Branch, Islamic Azad University, Lahijan, Iran.

Email: bafekry.asad@gmail.com and Email: mitragh@skku.edu



Fig. S1. (a) Possible stacking configurations formed by X(Al,In)Sb structures. Binding energy based on the interlayer distance for the most stable stacking configurations in (b) AlSb and (c) InSb.



Fig. S2. Electronic band structure of AlSb and InSb monolayers with a)PBE and b)HSE06 functional.