

Supplement material for: Optical Properties Enhancement via WSSe/Silicene Solar Cell Junctions

Renan Narciso Pedrosa,^{*a} Cesar E. P. Villegas^c, A.R.
Rocha^d, Rodrigo G. Amorim^b, and Wanderlã L. Scopel^a.

Phonon dispersion of the pristine structures

The Figs. S1-a and S1-b shows the phonon dispersion of WSSe and Silicene monolayers, respectively. The maximum optical phonon energy is approximately 51 meV for the Janus and 71 meV for the Silicene.

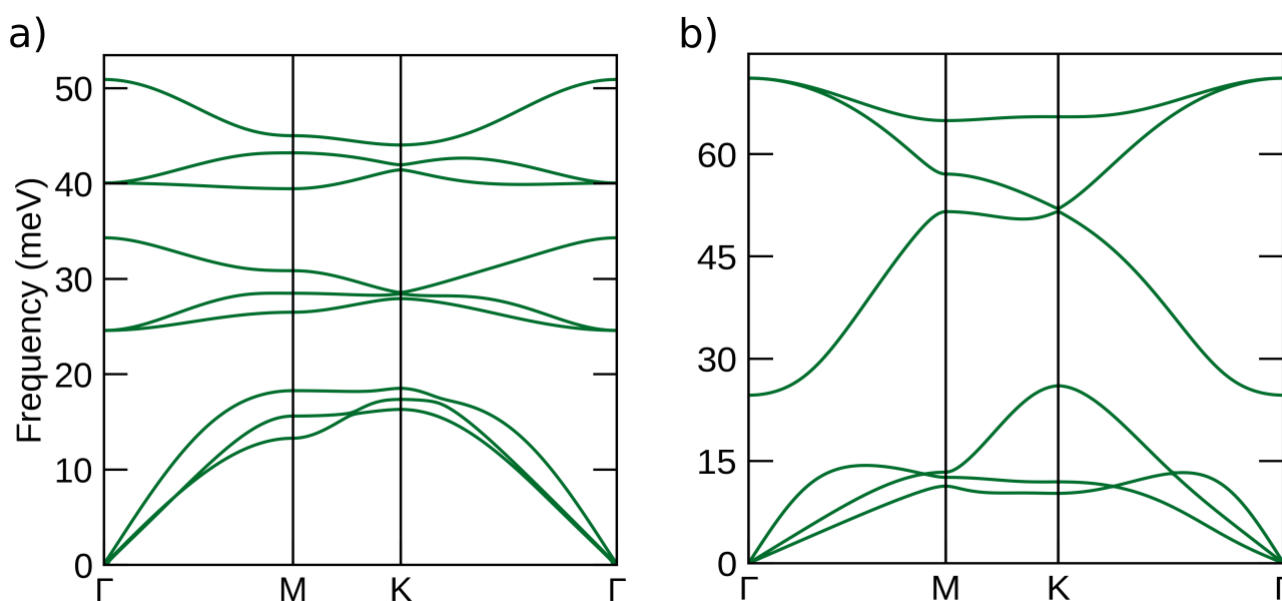


Fig. S1: Phonon dispersion of monolayer a) WSSe and b) Silicene.

^a Departamento de Física, Universidade Federal do Espírito Santo- UFES , Vitória/ES, Brazil; E-mail: renannarcisopedrosa@gmail.com

^b Departamento de Física, ICEx, Universidade Federal Fluminense - UFF, Volta Redonda/RJ, Brazil; E-mail: rgamorim@id.uff.br

^a Departamento de Física, Universidade Federal do Espírito Santo- UFES , Vitória/ES, Brazil; E-mail: wanderla.scopel@ufes.br

^c Departamento de Ciencias, Universidad Privada del Norte, Lima 15434, Peru; E-mail: cesar.perez@upn.edu.pe

^d Instituto de Física Teórica, Universidade Estadual Paulista (UNESP), Rua Dr. Bento T. Ferraz, 271, São Paulo, SP 01140-070, Brazil.;

E-mail:

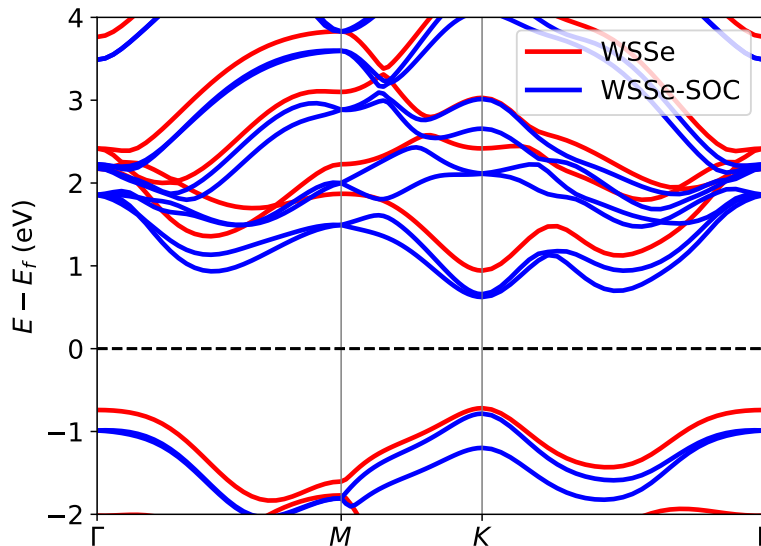


Fig. S2: Band structure of the Janus monolayer without SOC and with SOC.

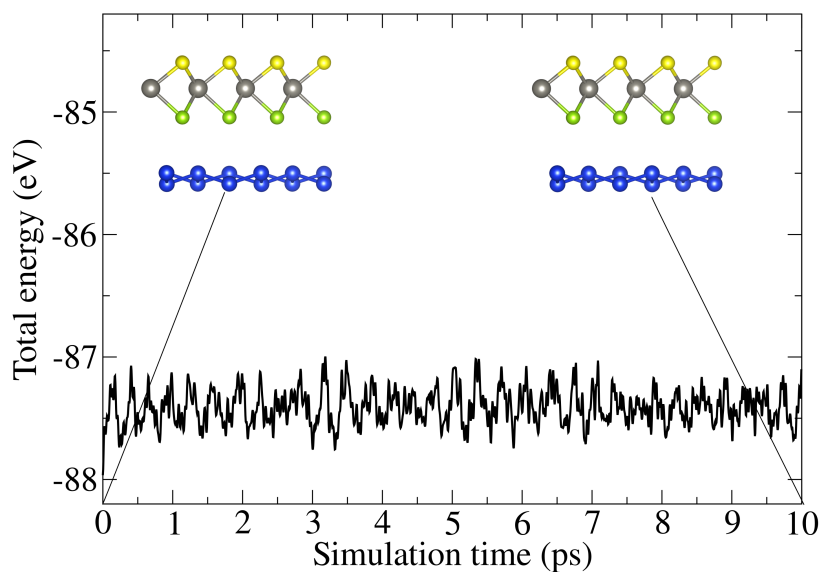


Fig. S3: Fluctuations of the total energy and Atomic geometries of the WSSe/Silicene heterostructure at 300K for 0 and 10 ps AIMD simulation.

BSE convergence tests

In Fig. S5 and S6 we present the convergence of the BSE parameters with respect to the energy cutoff in the exchange part of the BSE kernel, the energy cutoff of the screened Coulomb potential matrix in the e-h attractive

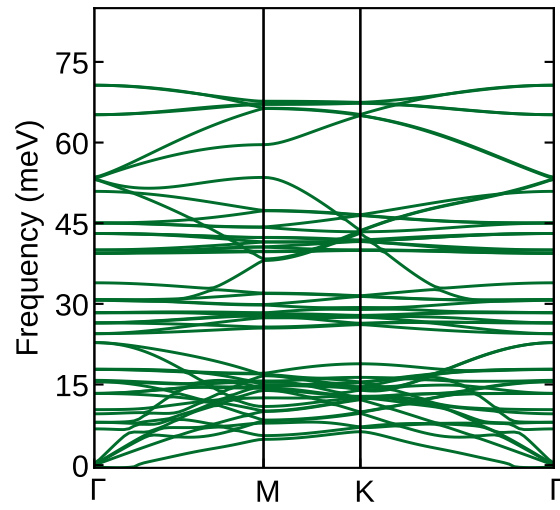


Fig. S4: Phonon dispersion of WSSe/Si heterostructure. The maximum optical phonon energy is approximately 71 meV.

Kernel, number of bands in the static screening and the k-grid sample.

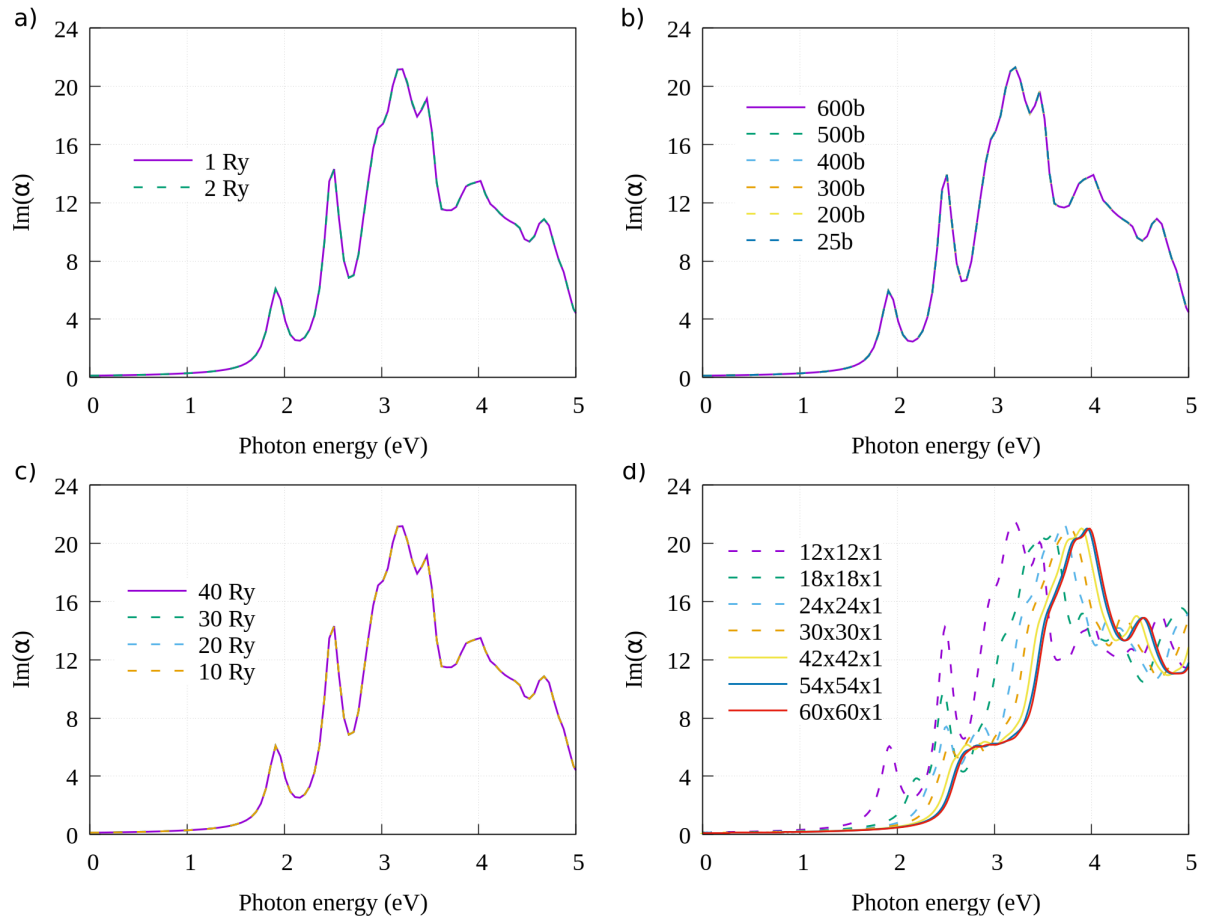


Fig. S5: Convergence BSE parameters of the WSSe monolayer

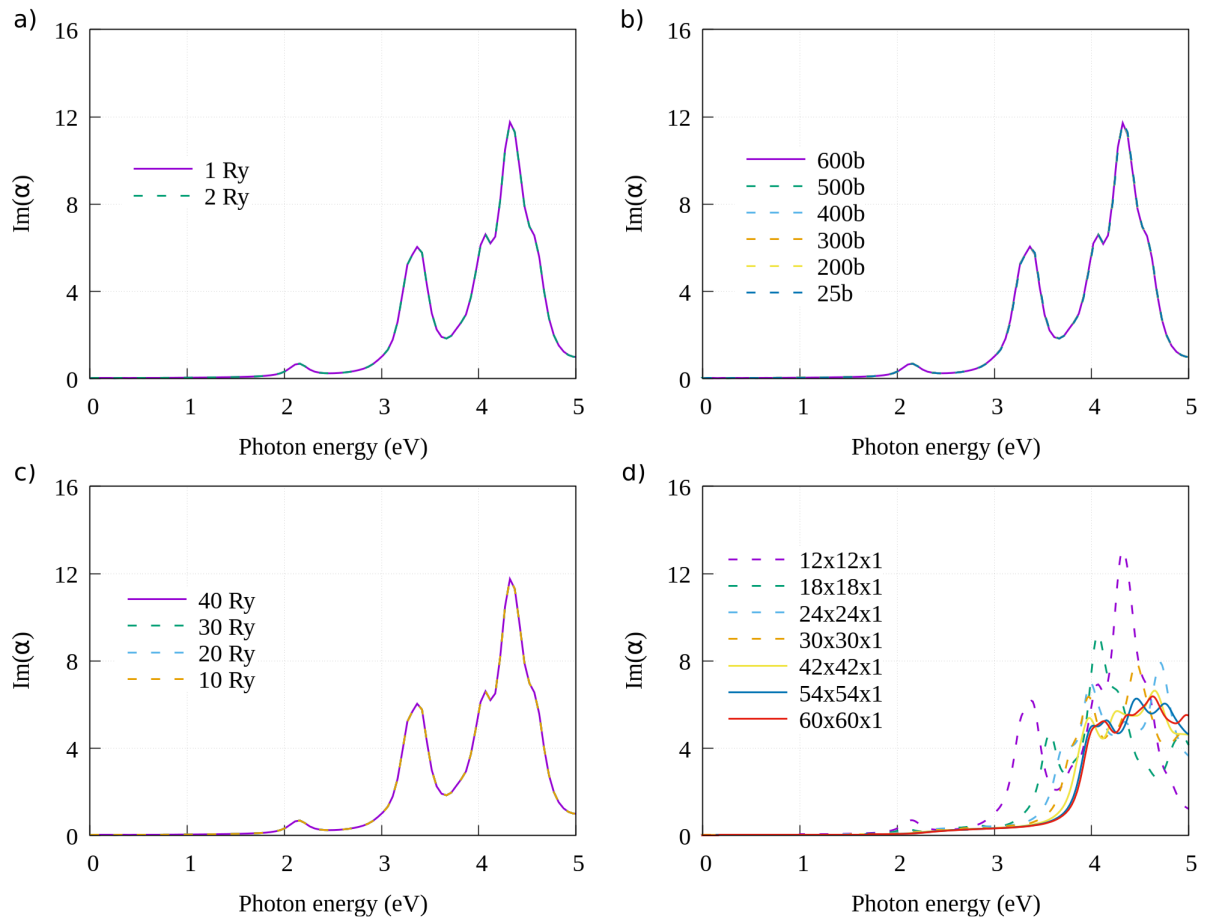


Fig. S6: Convergence BSE parameters of the Silicene monolayer