SUPPLEMENT

Supplementary Material for "Tuning the Electronic and Transport Properties of Penta-Graphene Nanoribbons by Creating Vacancies and Applying an External Electric Field"

M. Balvasi* and A. Avazpour

Physics Department, Faculty of Sciences, Yasouj University, Yasouj, Iran

Received: 21.10.2024 & Accepted: 16.01.2025

Doi: 10.12693/APhysPolA.147.124.S1 *e-mail: mohsen.balvasi@gmail.com

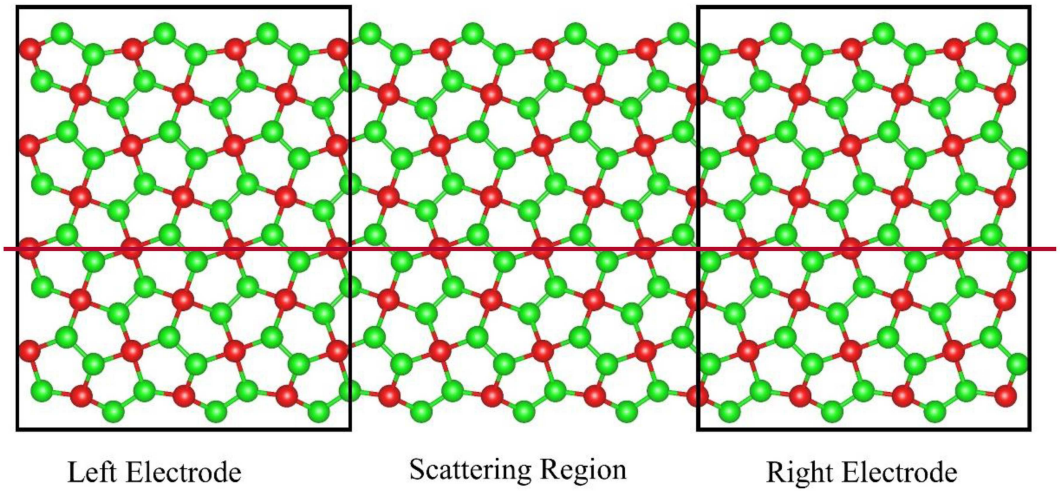

Fig. S1. Schematic illustration of the transport device. All three areas are of the same material.

TABLE SI

The energy gap, type of band gap, and electronic phase for all configurations when the single vacancy is created in all possible sites.

Single vacancy sites	Energy band gap [eV]	Type of band gap	Electronic phase
(1,1)	2.58	indirect	semiconductor
(1,2)	1.44	indirect	semiconductor
(1,3)	1.79	indirect	semiconductor
(1,4)	2.67	indirect	semiconductor
(1,5)	0.62	indirect	semiconductor
(1,6)	1.83	indirect	semiconductor
(1,7)	2.69	indirect	semiconductor
(1,8)	0.54	indirect	semiconductor
(1,9)	1.88	indirect	semiconductor
(1,10)	2.60	indirect	semiconductor
(1,11)	0.46	indirect	semiconductor
(1,12)	1.80	indirect	semiconductor

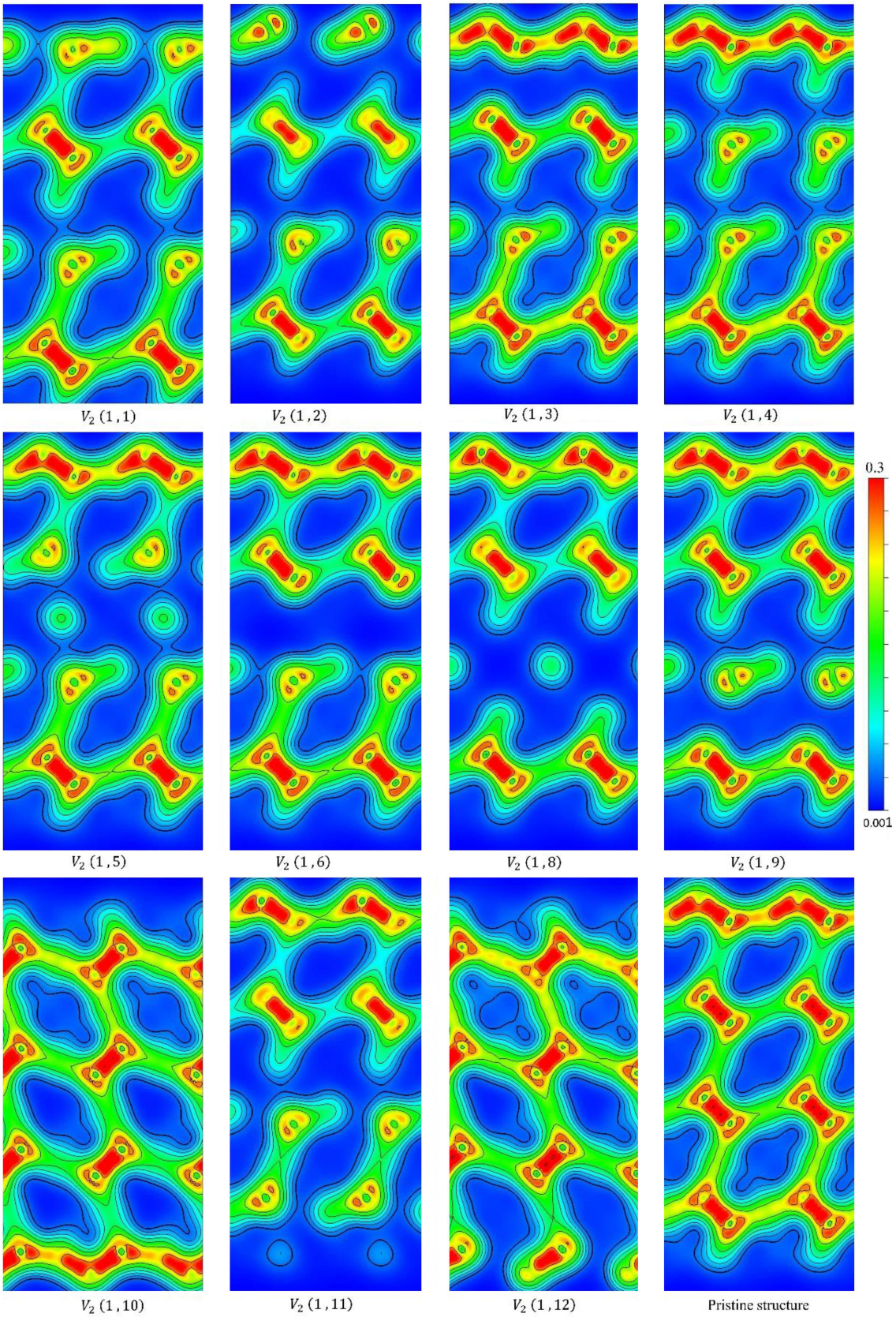

Fig. S2. The charge density distribution of sp_2-hybridized carbon atoms was analyzed using DFT calculations for all vacancy structures when the first vacancy is fixed at site $(1, 7)$. The results shown in this figure indicate that the cause of the change of electronic and transport properties with the creation of a vacancy in the structure is related to the modifications in the charge density of carbon atoms and the changes in their hybridization.

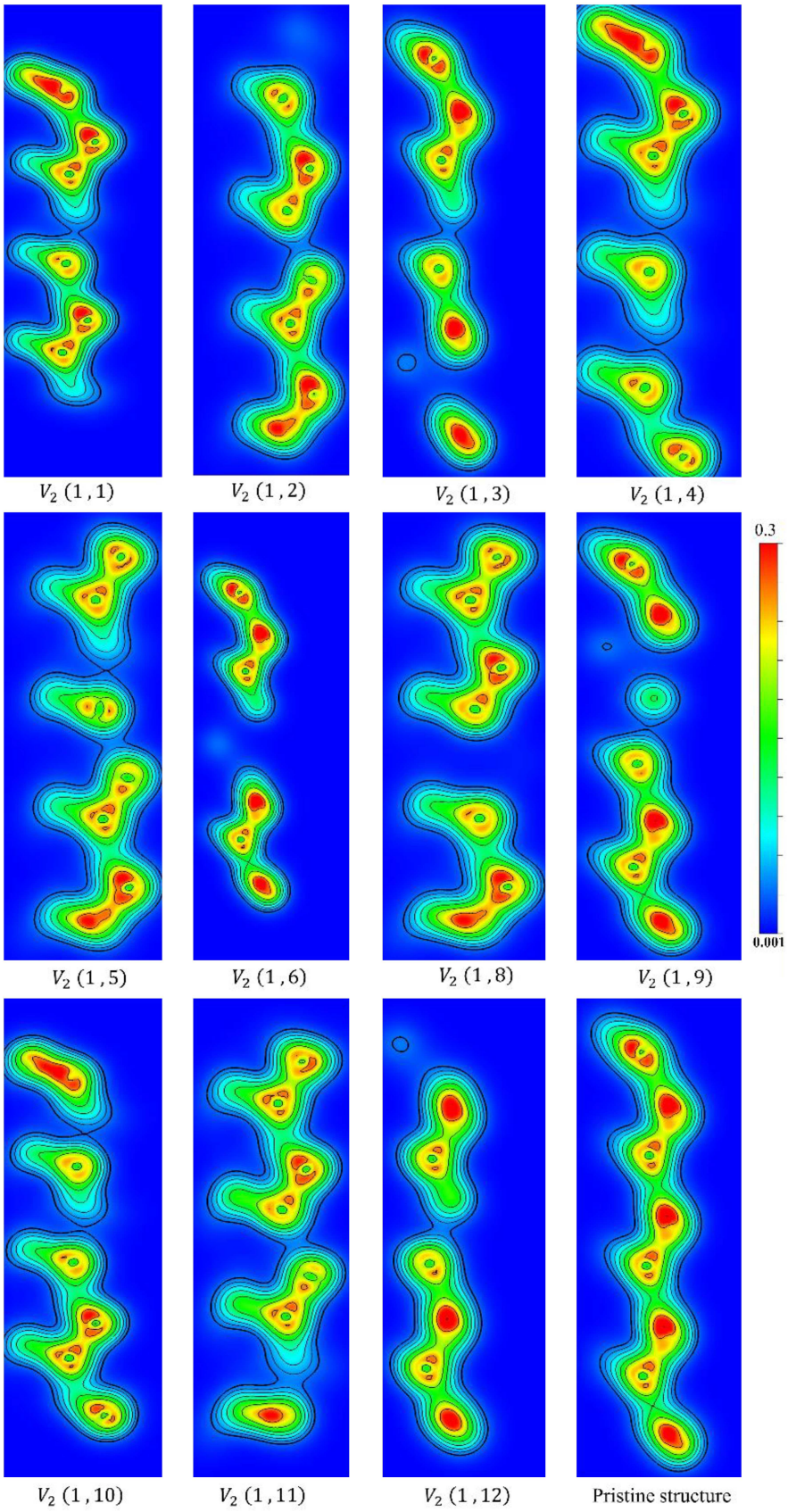

Fig. S3. The charge density distribution of sp_3-hybridized carbon atoms was analyzed using DFT calculations for all vacancy structures when the first vacancy is fixed at site $(1, 7)$. Analysis of the charge density diagrams of sp_2- and sp_3-hybridized carbon atoms shows that the charge density in sp_3 bonds is lower than in sp_2 bonds. This difference indicates a stronger interaction in sp_2 bonds compared to sp_3 bonds.

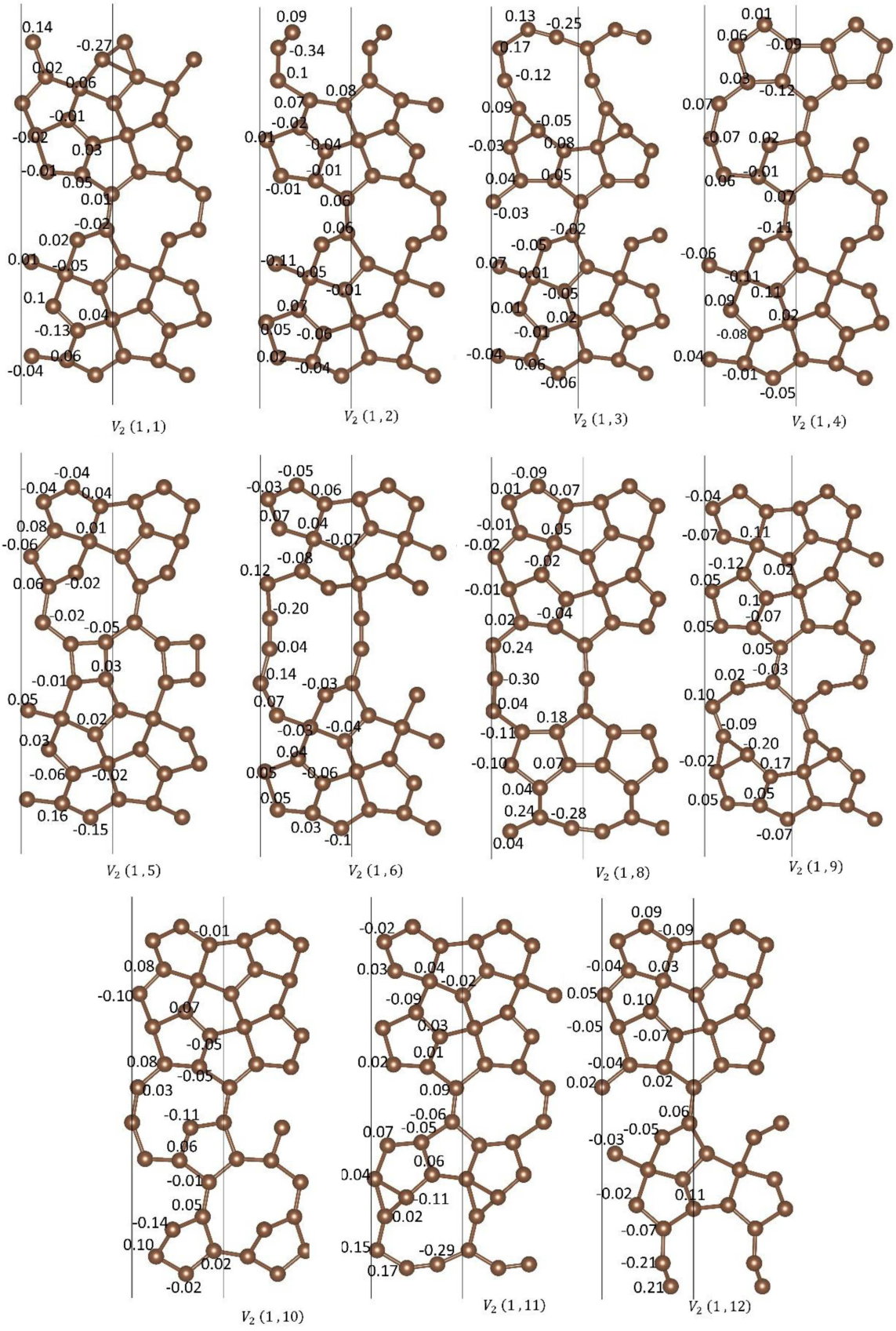

Fig. S4. Calculation of effective charge transfer between carbon atoms due to double vacancy effect using Bader's charge analysis method. The effective charge transfer depends on vacancy structures; all atoms are reconstructed due to dangling bonds around the vacancies. These reconstructions change the hybridization and atomic contribution of carbon atoms near the vacancies.