Electronic Supplementary Material (ESI) for RSC Advances.

Bandgap Engineering of Germanene for Gas Sensing Applications

Ong Kim Le[1,2], Viorel Chihaia[3], Do Ngoc Son[4,5,*]

[1]*Institute of Fundamental and Applied Sciences, Duy Tan University, Ho Chi Minh City, 700000, Vietnam.*

[2]*Faculty of Natural Sciences, Duy Tan University, Da Nang City, 550000, Vietnam.*

[3]*Institute of Physical Chemistry "Ilie Murgulescu" of the Romanian Academy, Splaiul Independentei 202, Sector 6, 060021 Bucharest, Romania.*

[4]*Ho Chi Minh City University of Technology (HCMUT), 268 Ly Thuong Kiet Street, District 10, Ho Chi Minh City, Vietnam.*

[5]*Vietnam National University Ho Chi Minh City, Linh Trung Ward, Ho Chi Minh City, Vietnam.*

[*]*E-mail: dnson@hcmut.edu.vn*

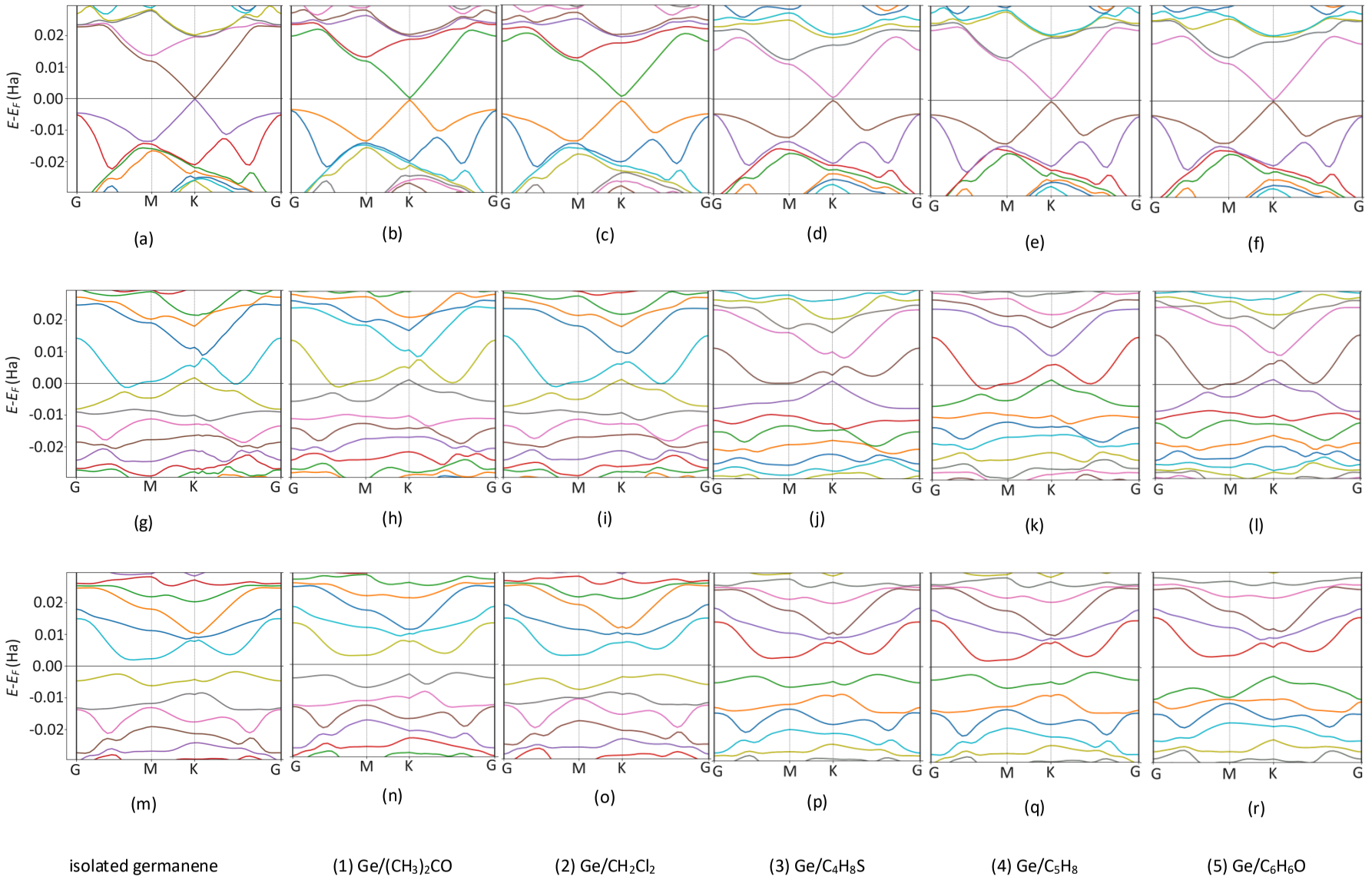

Figure S1. The band structure of germanene before and after the VOC adsorption by PBE+vdW-DF2 method. Perfect (top panel), Vacancy-1 (middle panel), and Vacancy-2 (bottom panel). The Fermi level at 0 Ha.

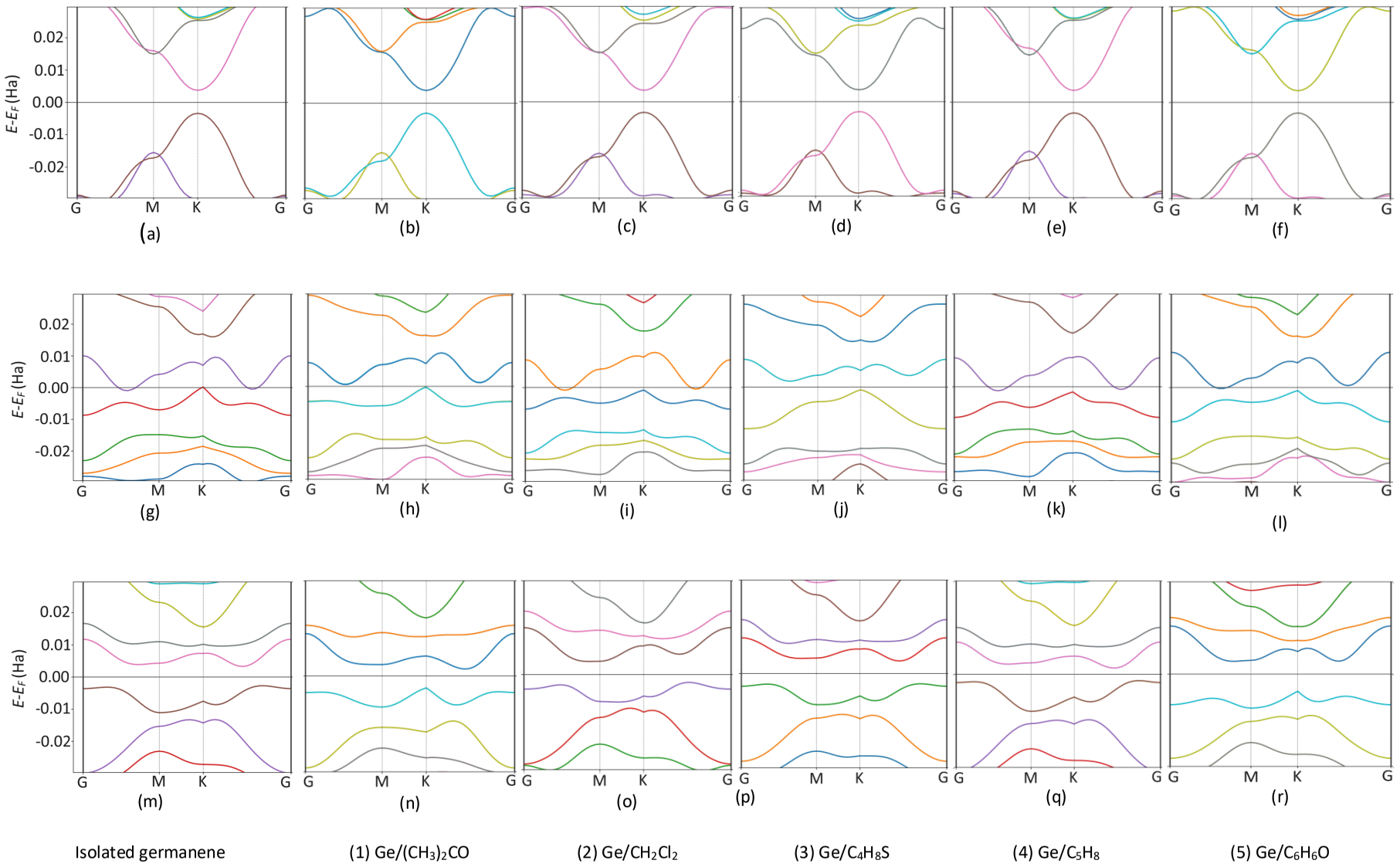

Figure S2. The band structure of germanene before and after the VOC adsorption by PBE+HSE06 method. Perfect (top panel), Vacancy-1 (middle panel), and Vacancy-2 (bottom panel). The Fermi level at 0 Ha.