Electronic Supplementary Material (ESI) for RSC Advances.

Exploring silicene monolayer as promising sensor platform to detect and capture NO and CO gas

Duy Khanh Nguyen,[1] Duc-Quang Hoang,[2] and D. M. Hoat[3,4,*]

[1]Group of Computational Physics and Simulation of Advanced Materials, Institute of Applied Technology, Thu Dau Mot University, Binh Duong Province, Vietnam

[2]Applied Computational Civil and Structural Engineering Research Group, Faculty of Civil Engineering, Ton Duc Thang University, Ho Chi Minh City, Viet Nam

[3]Computational Laboratory for Advanced Materials and Structures, Advanced Institute of Materials Science, Ton Duc Thang University, Ho Chi Minh City, Viet Nam

[4]Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Viet Nam

*Coresponding author: dominhhoat@tdtu.edu.vn

Table S1: Adsorption energy (eV/molecule) of XO (X = N and C) molecules onto pristine and Al-doped silicene monolayer calculated with LDA functional.

	XO	2XO1	2XO2	2XO3	2XO4	3XO	4XO
	Onto pristine silicene						
NO	-0.89	-2.00	-0.89	-0.79	-0.86	-0.93	-0.90
CO	-0.22	-0.81	-0.28	-0.13	-0.27	-0.28	-0.29
	Onto Al-doped silicene						
CO	-0.78	-1.13	-0.79	-0.82	-0.78	-0.82	-0.82

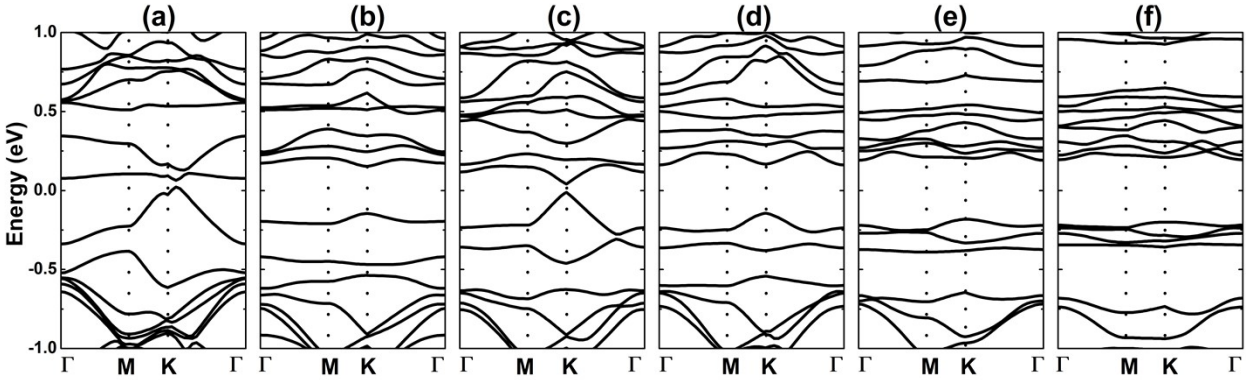

Figure S1. Electronic band structure (a) 2CO1-, (b) 2CO2-, (c) 2CO3-, (d) 2CO4-, (e) 3CO- and (f) 4CO-adsorbed silicene monolayer.

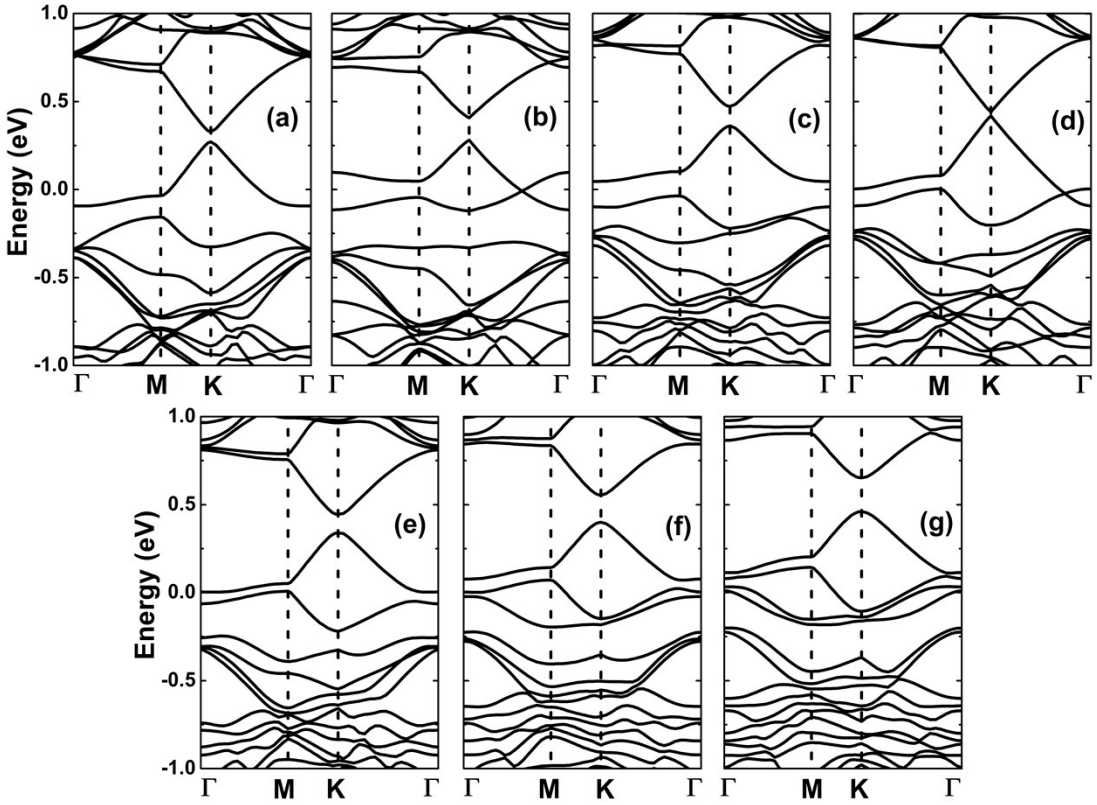

Figure S2: Band structure of (a) Al-, (b) 2Al1-, (c) 2Al2-, (d) 2Al3-, (e) 2Al-4, (f) 3Al-, and (g) 4Al-doped silicene monolayer.