Carbon monoxide sensing properties of Ga, Al and B-doped Si nanowires

José E. Santana[a], Francisco de Santiago[a], Alejandro Trejo[a], Alvaro Miranda[a*], Eliel Carvajal[a], Luis A. Pérez[b] and Miguel Cruz-Irisson[a]

[a] *Instituto Politécnico Nacional, ESIME-Culhuacán, Av. Santa Ana 1000, C.P. 04430, Ciudad de México, México;*
[b] *Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 Ciudad de México, México*

Silicon nanowires (SiNWs) have been considered as potential chemical sensors due to their large surface-to-volume ratio; besides, the possible integration of several nanowires into arrays allows to visualize those as sensors. Because of that, SiNWs have been studied as sensors of harmful gases, such as CO, NO, NO_2 and SO_2 [1, 2]. However, doping SiNWs could influence their sensing capacity, and this influence has not been reported yet in literature. For this work, we studied theoretically the surface adsorption of a CO molecule on hydrogen-passivated silicon nanowires (H-SiNWs), grown along the [111] crystallographic direction, as well as on a SiNW with a dangling bond. To analyze the doping effects on the H-SiNWs' chemical sensing properties, we considered three nanowire diameters, and studied the effect of B-, Al-, and Ga-doping, on the adsorption of CO, by Density Functional Theory calculations. The results indicate that molecular CO adsorbs more strongly onto the B-doped H-SiNW than on the pristine H-SiNW. The following trend is observed for the CO adsorption energies: E_{ads}[B-doped] > E_{ads}[Al-doped] > E_{ads}[Ga-doped] > E_{ads}[undoped], for all diameters. The electronic charge transfers between the SiNWs and the adsorbed CO were estimated by using both the Hirshfeld and Voronoi population analysis. The CO adsorbed onto the undoped H-SiNWs has an electron-acceptor character, while the CO adsorbed onto the B-, Al-, and Ga-doped H-SiNWs exhibits an electron-donor character.

[1] A. Miranda, F. de Santiago, L.A. Pérez, and M. Cruz-Irisson, Silicon nanowires as potential gas sensors: A density functional study, *Sensors and Actuators B: Chemical* **242** (2017) 1246-1250.
[2] F. de Santiago, A. Miranda, A. Trejo, E. Carvajal, M. Cruz-Irisson, and L.A. Pérez, Chemical sensing in silicon nanowires: quantum confinement effects, *Journal of Molecular Modelling* (Submitted).

Acknowledgments
This work was supported by IPN-SIP project 20170885 and multidisciplinary projects 2016-1770 and 2016-1771; PAPIIT-DGAPA-UNAM IN107717. Computing resources were given by project LANCAD-UNAM-DGTIC-180. J. E. Santana and F. de Santiago would like to thank the CONACYT and BEIFI-IPN for their scholarships. L.A. Pérez acknowledges partial support from "Cátedra Marcos Moshinsky".

* E-mail: amirandad.ipn@gmail.com