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Computational modelling of the Li effects on the electronic structure of porous silicon[1] MARÍA LUCERO GOMEZ-HERRERA, Facultad de Ingeniería Universidad Autónoma de Querétaro C. P. 76000, México Querétaro, ÁLVARO MIRANDA DURÁN, ALEJANDRO TREJO BAÑOS, MIGUEL CRUZ IRISSON, Instituto Politécnico Nacional, ESIME Culhuacan, Av. Santa Ana 1000 C, P. 04918 México D. F. — This work analyses the effects of Li impurities on the electronic structure of pSi by means of the density functional theory with the generalized gradient approximation and the supercell scheme. The porous structures were modeled by removing atoms in the [001] direction of an otherwise perfect Si crystal. All surface dangling bonds were saturated with H atoms. To model the Li impurities some H atoms are replaced with Li atoms at the surface. Results show additional bands around the Fermi level with the insertion of a single Li atom on the pore surface, which suggests a trap-like state of localized charge. With increasing concentration of surface Li the band gap gradually decreases approaching to a metallic behavior. This results could be important to the application of pSi in Li-ion batteries

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