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Electrocatalytic property of PtBi and PtPb line compounds via DFT¹ LIN-LIN WANG, D. D. JOHNSON, Department of Materials Science and Engineering and the Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign — A major obstacle to practical, mass market fuel cell (e.g. hydrogen and direct methanol) technology is CO poisoning of Pt anode. Pt alloys, such as disordered $\text{Pt}_x\text{Ru}_{(1-x)}$, are known to have an increased CO-tolerance. There has been significant effort to understand the mechanism for increased CO-tolerance and to design better catalyst via alloyed nanoparticles and surface alloys. Alternatively, Pt intermetallic compounds, such as with Bi and Pb, have been observed to improve dramatically the CO-tolerance. [E. Casado-Rivera et al. ChemPhysChem 4, 193 (2003) and J. Am. Chem. Soc. 126, 4043 (2004)] Here we use density functional theory to study the adsorptions of CO, H and OH on these materials. We find that (100) and (110) surfaces of PtBi and PtPb line compounds have lower cleavage energy than (001) surface. Adsorption energies and electronic structure are examined to explain the increased CO-tolerance.

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