Electrocatalytic property of PtBi and PtPb line compounds via DFT

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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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