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The role of Ga in the acetylene hydrogenation on PdGa intermetallic

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Density functional theory calculations were performed, studying the acetylene hydrogenation reaction over the PdGa(110) surface. The reaction C2H2+H2⟶ C2H4 was simulated and characterized in terms of the change in the chemical bonding. Also we analyze the changes in the electronic structure in the different steps of the reaction, what allowed us to understand more the role of Pd, Ga, and C2H2 during the reaction. This analysis, together with the determination of the bond order in each step of the reaction, revealed that Ga is a part of the active site and not a single spacer.

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