Supporting Information

First-principles study of the effect of compressive strain on oxygen adsorption in Pd/Ni/Cu-alloy-core@Pd/Ir-alloy-shell catalysts

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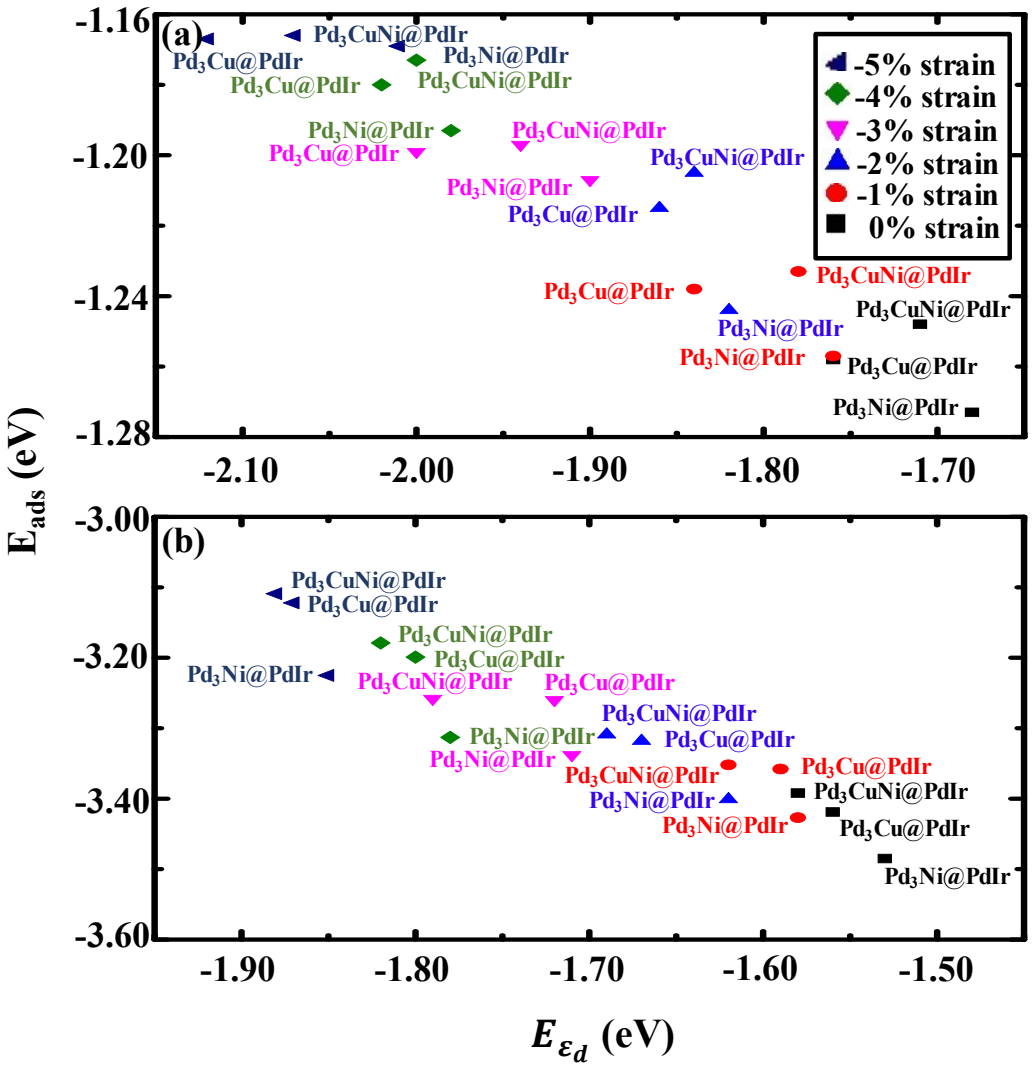

Figure S1. Dioxygen-adsorption energy as a function of d-band center for (a) surface Pd and (b) surface Ir at different compressive strains. This figure clearly demonstrates lower dioxygen binding to the catalyst surface with increasing compressive strain and d-band center downshift. Individual catalysts are labelled according compressive strain for clarity.

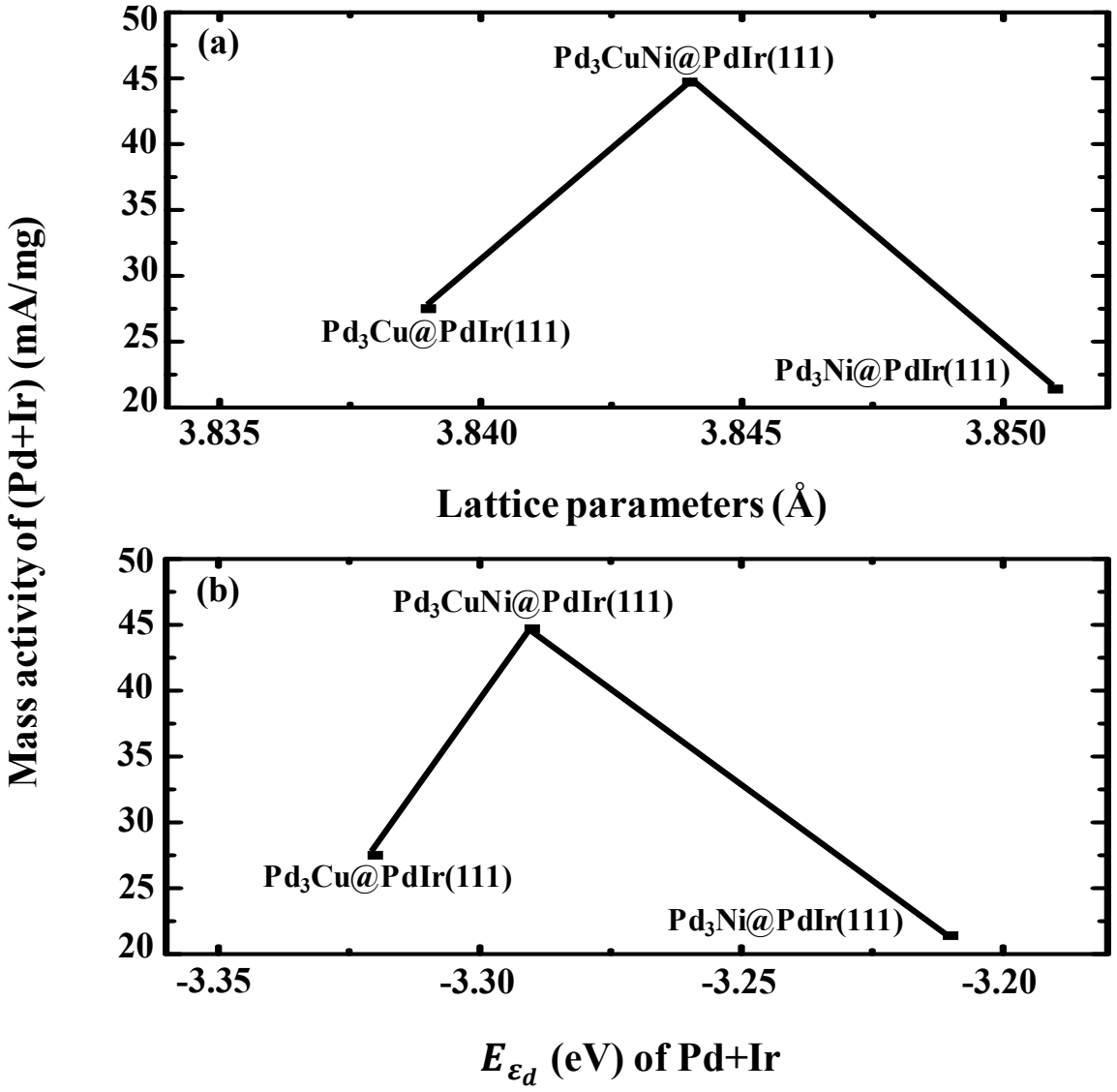

Figure S2. Volcano plots based on the experimentally obtained mass activity as a function of: (a) experimentally determined lattice parameter and (b) theoretically calculated d-band center value for the Pd and Ir surfaces. Both figures show similar trends, with the Pd_3CuNi@PdIr catalyst at the apex of the volcano, the Pd_3Cu@PdIr catalyst at the left-hand side and the Pd_3Ni@PdIr catalyst at the right-hand side of the apex. Note: the black lines are provided for guidance purposes.