Supplementary information

Palladium phosphide modified three-dimensional phospho-doped graphene materials for hydrogen storage

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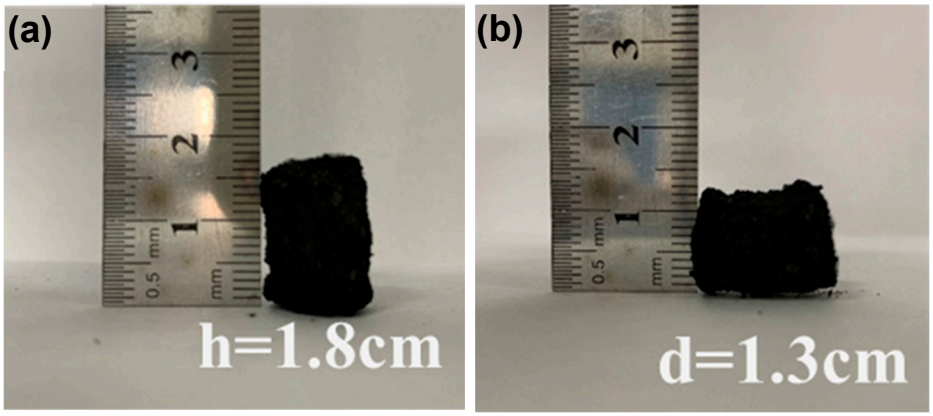


Figure S1: (a-b) Optical images of 3D Pd_3P/P-rGO-Y. (Y=300, 500, 700, 900)

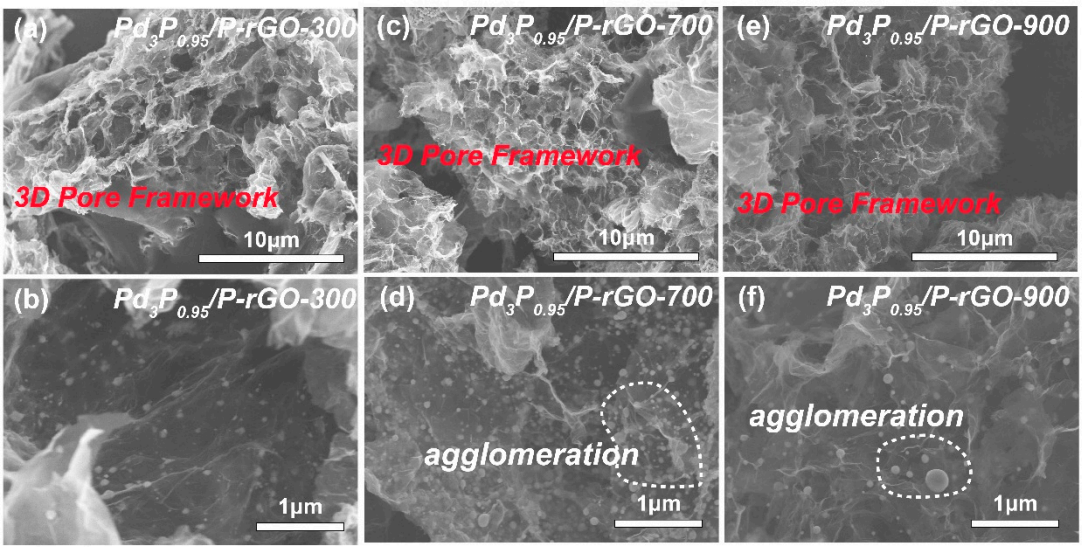


Figure S2: SEM images of 3D $Pd_3P_{0.95}$/P-rGO prepared at different thermal reduction temperatures: (a-b) $Pd_3P_{0.95}$/P-rGO-300, (c-d) $Pd_3P_{0.95}$/P-rGO-700, (e-f) $Pd_3P_{0.95}$/P-rGO-900.

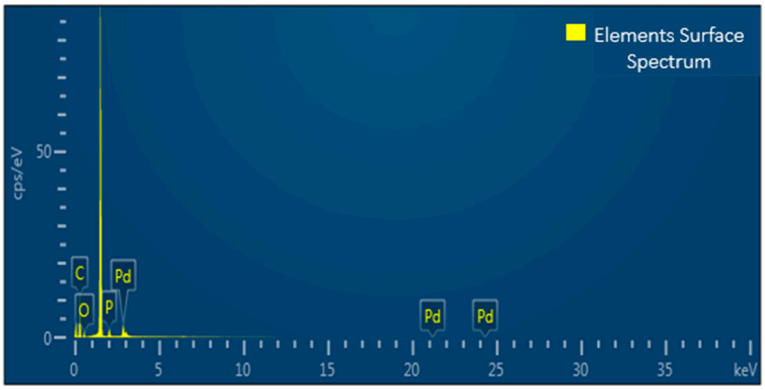


Figure S3: Energy Dispersive X-Ray Analysis (EDX) of the sample to confirm successful doping of P in the $Pd_3P_{0.95}$/P-rGO

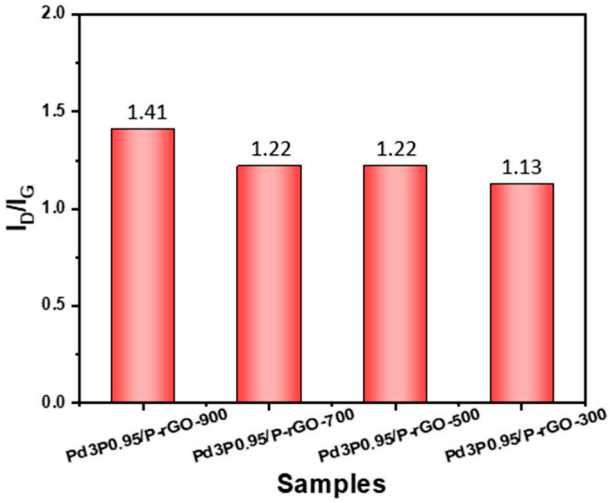


Figure S4: Statistical chart of I_D/I_G values.

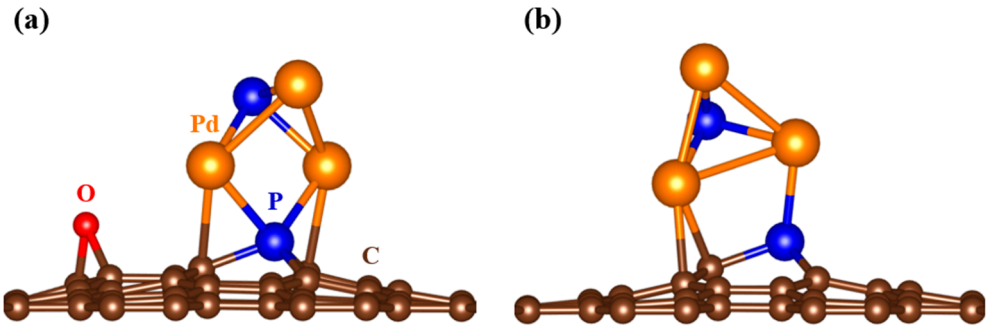


Figure S5: Optimized structure of (a) Pd_3P/P-rGO and (b) Pd_3P/P-G.

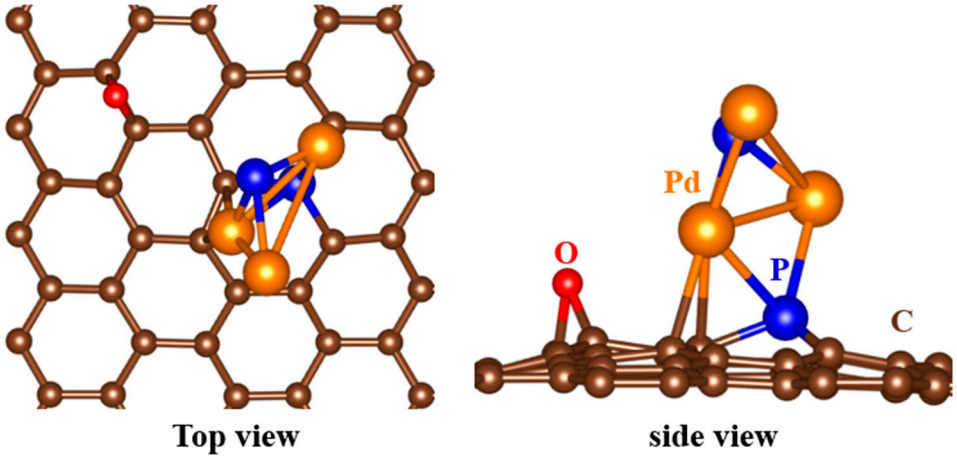


Figure S6: Molecular Dynamics snapshot of Pd_3P/P-rGO at 300K after 1 ps. The structure appears to be stable and there are minimal changes in C-C bond length.