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Anchoring platinum on graphene using metallic adatoms F.G. SEN, Department of Mechanical, Automotive and Materials Engineering, University of Windsor, Windsor, ON, Canada, Y. QI, Chemical Sciences and Materials Systems Laboratory, General Motors R&D Center, Warren, MI U.S.A., A.T. ALPAS, Department of Mechanical, Automotive and Materials Engineering, University of Windsor, Windsor, ON, Canada — To anchor Pt on the graphene surface 25 different metallic adatoms were individually inserted into Pt(111)/graphene interface and the work of separation required to break the interface between Pt-adatom and C-adatom bonds were computed using first principles calculations. With the exception of Al, Zn and Au, all metals increased the strength of the Pt/graphene interface, while many transition metals with unfilled d orbitals, such as Sc, Ti, V, Cr, Co, Ni, Zr, Nb, Mo, Ru, Rh, Ta, W, Re, Os, Ir, could increase the Pt/graphene interface strength from 0.009 J/m^2 to above 0.5 J/m^2. The Pt-adatom bond had metallic character and its strength was proportional to the amount of charge transferred from the adatom to the Pt. The strength of carbon-adatom bond was proportional to the ratio of charge transferred to the carbon over charge transferred to the platinum from the adatom. As this ratio was >1.0 for Ir, Os, Ru, Rh and Re and these emerged as the most promising adatoms for anchoring Pt on graphene.

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