Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Surface Phase Diagram and Thermodynamic Stability of Functionalisation of Nanodiamonds†

Lin Lai,[*a] **Amanda S. Barnard**[a]

Supplementary Information

Figure 1 and Figure 2 present the formation energies of H- and O-passivation and OH-functionalisation, as a function of the partial pressure ($\log(P/P_0)$) for the C_{705} and C_{837} nanodiamonds, respectively. The former is calculated at $T = 1123.15$ K, and the latter at $T = 298.15$ K.

Figure 3, Figure 4 and Figure 5 presents the temperature-dependent stability for H-passivated, O-passivated and OH-functionalised C_{705} and C_{837} nanodiamonds, respectively (at atmospheric pressure). The details of these results can be found in reference 1.

References

1 L. Lai and A. S. Barnard, *Nanoscale*, 2011, **3**, 2566–2575.

[a] *CSIRO Materials Science and Engineering, Parkville, VIC, 3052, Australia. Fax: +61-3-9662-7145; Tel: +61-3-9662-7356; E-mail: amanda.barnard@csiro.au*

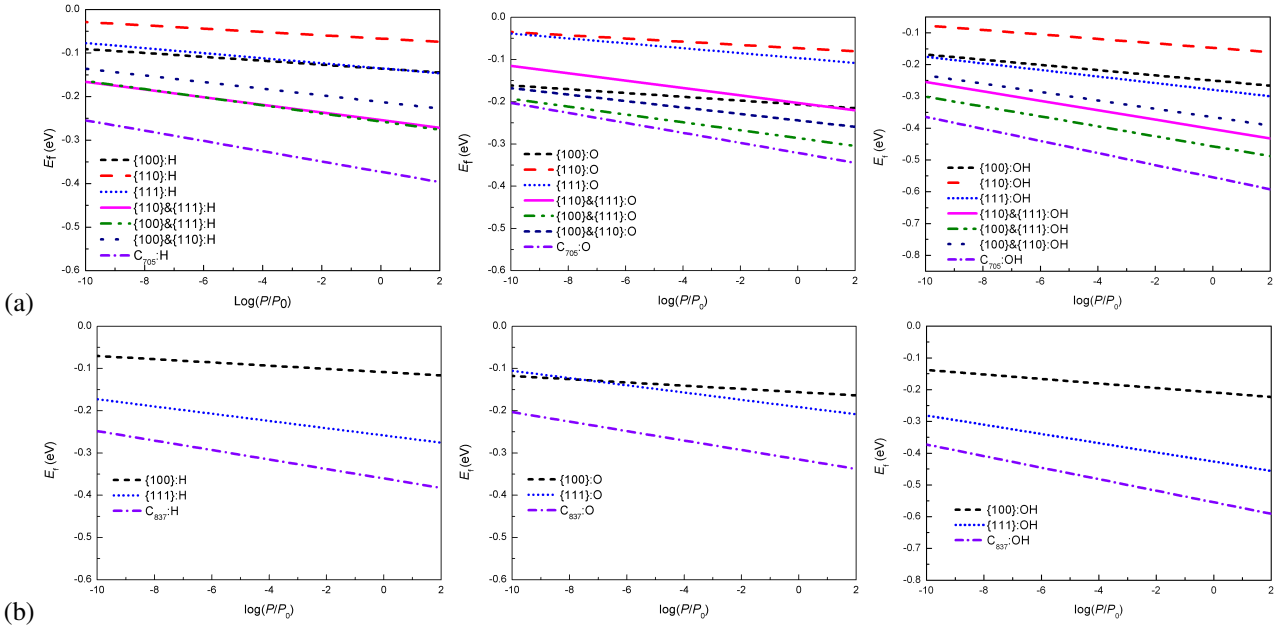

Fig. 1 Formation energy versus partial pressure (log(P/P_0)) for C_{705} (upper) and C_{837} (lower) nanodiamonds at T=1123.15 K.

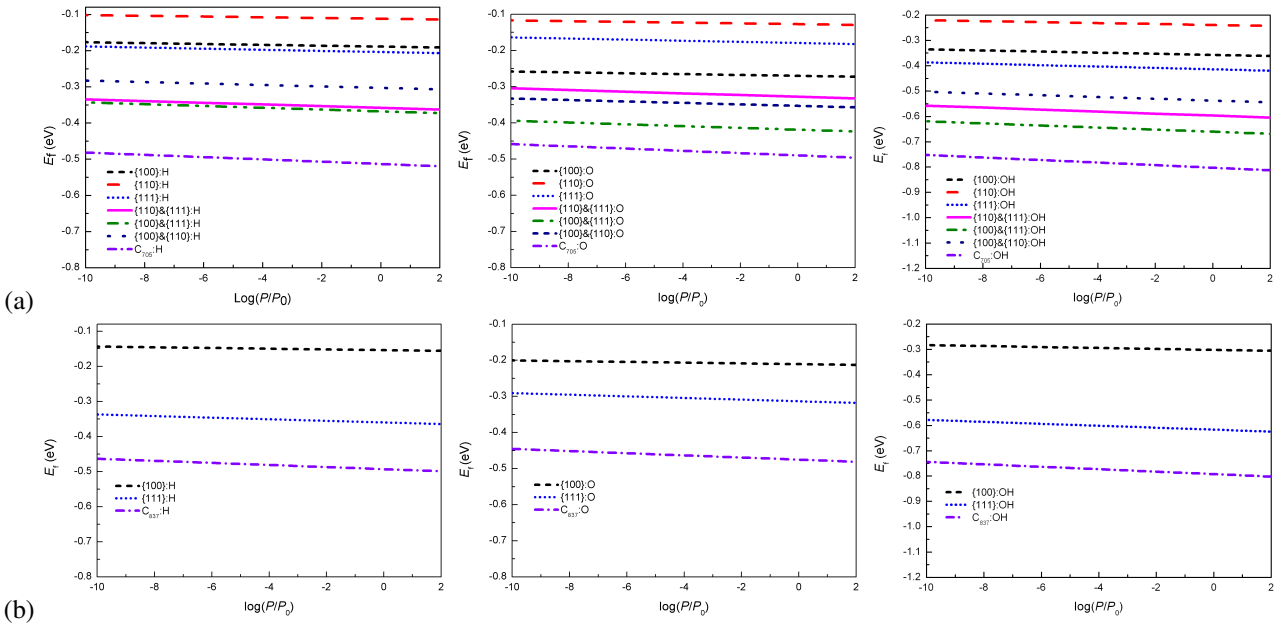

Fig. 2 Formation energy versus partial pressure (log(P/P_0)) for C_{705} (upper) and C_{837} (lower) nanodiamonds at T=298.15 K.

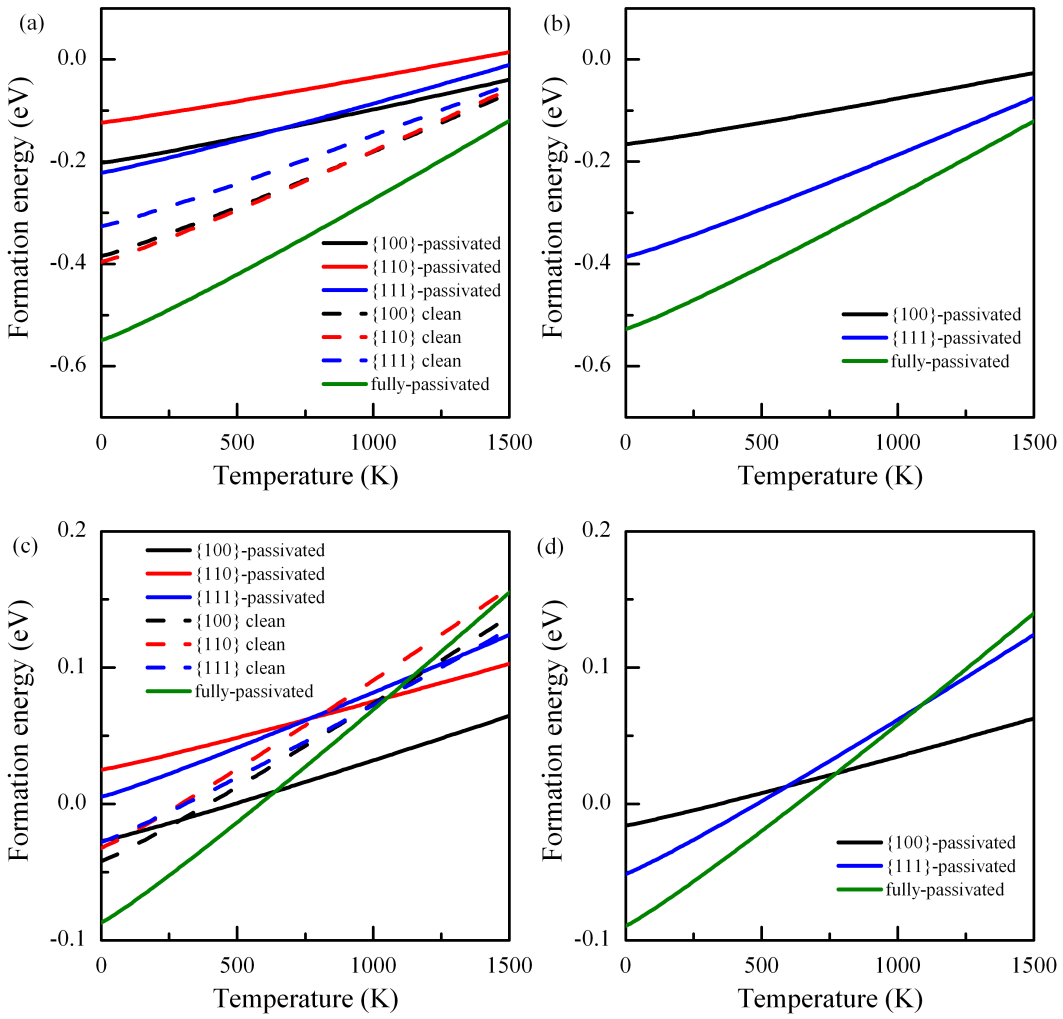

Fig. 3 Formation energy versus temperatures for H-passivated C_{705} (left) and C_{837} (right) nanodiamonds at a pressure of 1 atm.

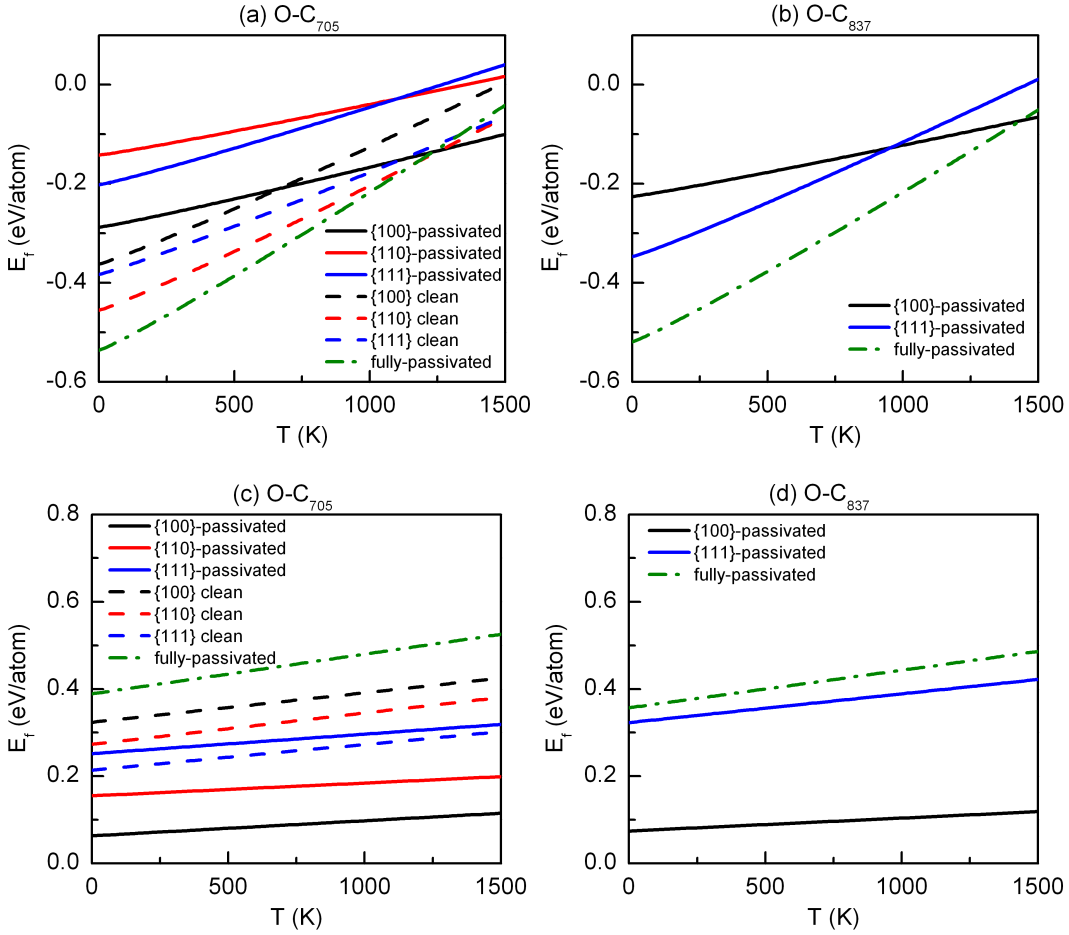

Fig. 4 Formation energy versus temperatures for O-passivated C_{705} (left) and C_{837} (right) nanodiamonds at a pressure of 1 atm.

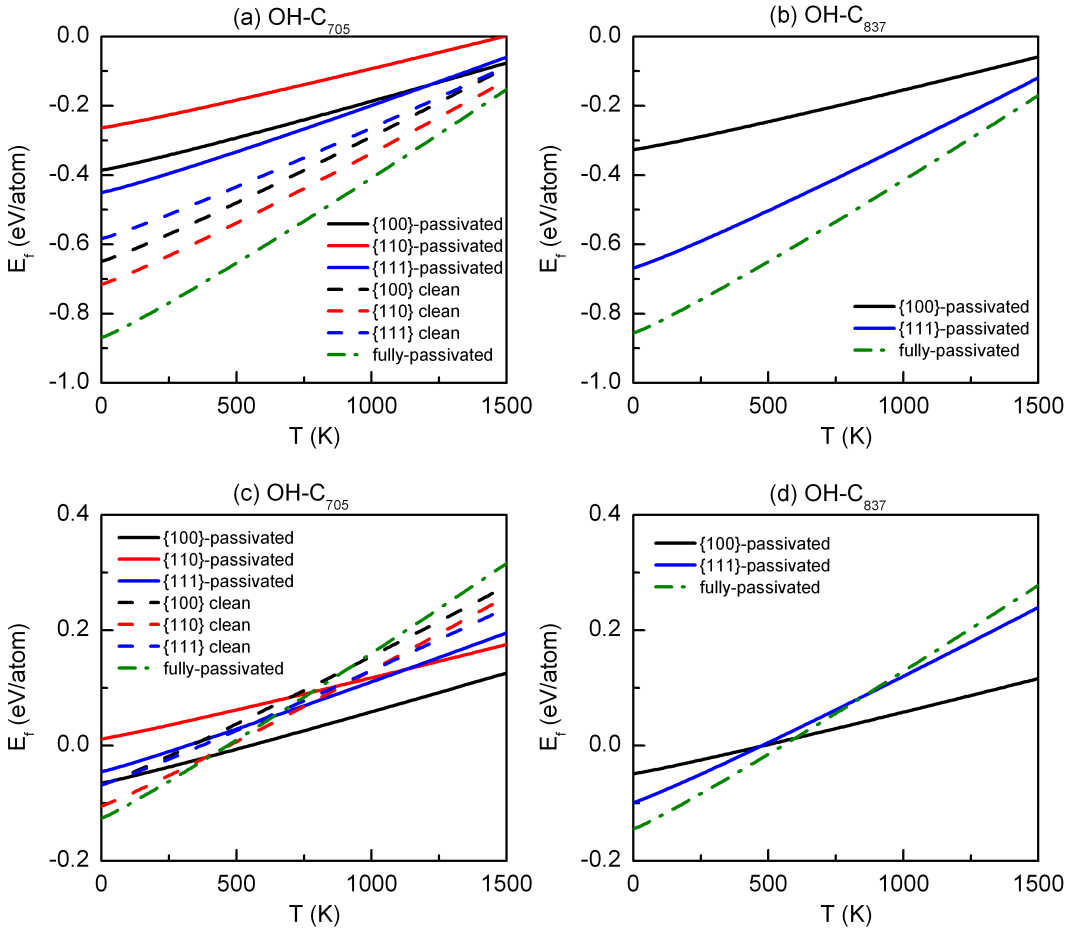

Fig. 5 Formation energy versus temperatures for OH-functionalised C_{705} (left) and C_{837} (right) nanodiamonds at at a pressure of 1 atm.