PDoS for Graphene-B<sub>4</sub>C<sub>3</sub> by HSE06 Total PDoS PDoS for Carbon in Graphene 10 2.5 Fermi energy -0.378 (eV) Fermi energy -0.378 (eV) (b) (a) Total PDoS Total PDoS  $s \; \mathrm{PDoS}$  $s \; \mathsf{PDoS}$  $p_x$  PDoS  $p_x$  PDoS  $p_y$  PDoS  $p_y$  PDoS 2.0 8  $p_z$  PDoS  $p_z$  PDoS --- Fermi energy --- Fermi energy Density of states 1.5 0.0\_6 PDoS for Boron in B<sub>4</sub>C<sub>3</sub> PDoS for Carbon in B<sub>4</sub>C<sub>3</sub> 2.5 2.5 Fermi energy -0.378 (eV) Fermi energy -0.378 (eV) (d) (c) Total PDoS Total PDoS  $s \; \mathsf{PDoS}$  $s \; \mathsf{PDoS}$  $p_x$  PDoS  $p_x$  PDoS  $p_y$  PDoS  $p_y$  PDoS 2.0 2.0  $p_z$  PDoS  $p_z$  PDoS --- Fermi energy --- Fermi energy Density of states

1. ... 1.5 1.0 0.5 0.5 -40 Energy (eV) Energy (eV)