Density functional theory (DFT)   oxygen functionalized graphene oxide

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.   CCS (Carbon dioxide Capture and Storage)

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,   graphene, CNT   . Graphene
,   activated carbon
.   graphene
,   density functional theory   molecular
simulation   .   (epoxy, hydroxyl)   graphene
oxide   .   graphene oxide   ,
                    binding energy   . Pristine graphene   graphene oxide
          binding energy
.   , DFT   modified   graphene

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