Graphene & Defected Graphene

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| d (Å) | Pristine | Defected |
|  |  |  |
| G | - | - |
| G\_CO2top | 1.599 | 1.499 |
| G\_CO2bridge | 4.288 | 4.312 |
| G\_CO2hole | 4.089 | 1.5 |

|  |  |  |  |  |
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| Ef (eV) | Pristine | | Defected | |
|  | k-poit(5 5 1) | k-poit(10 10 1) | k-poit(5 5 1) | k-poit(10 10 1) |
| G | 0.0976 | 0.0995 | -0.5114 | -0.5062 |
| G\_CO2top | 0.4315 | 0.4107 | 0.0575 | 0.0527 |
| G\_CO2bridge | 0.7766 | 0.7766 | 0.1098 | 0.0797 |
| G\_CO2hole | 0.7723 | 0.7723 | 0.0579 | 0.0532 |

|  |  |  |
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| Etot (Ry) | Pristine | Defected |
| G | -223.71470484 | -210.70968295 |
| G\_CO2top | -300.71788953 | -288.05063612 |
| G\_CO2bridge | -300.95623741 | -287.95140479 |
| G\_CO2hole | -300.95602031 | -288.05058188 |