Table 1. The calculated Gibbs energy of reaction for calcium carbonate hydrates

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Reactions | (eV) | (eV) | (eV) | (eV/atom) |
| CaCO3+1/2H2O=CaCO3·1/2H2O | -21652.643712 | -2471.826408 | -468.828781 | -0.052 |
| CaCO3+1H2O=CaCO3·1H2O | -26469.875901 | -2471.826408 | -468.828781 | -0.055 |
| CaCO3+6H2O=CaCO3·6H2O | -21152.058167 | -2471.826408 | -468.828781 | -0.139 |

Table 2. Lattice constant, volume of calcium carbonate hydrates accompanied with the available theoretical (DFT calculations) and experimental values

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Species | Structure | Spaces groups | Lattice constants(Å) | | |  | *ρ*(g.cm-3) | *V*(Å3) |  | | |
|  |  |  | a | b | c | *β* |  |  |  | | |
| CaCO3·1/2H2O | Monoclinic | P121/c1(14) | 9.64 | 10.47 | 6.42 | 89.967 | 2.415 | 649.31 | This work | | |
|  |  |  | 9.33 | 10.43 | 6.16 | 90.520 | 2.416 | 600.02 | | | Exp. value[8] | |
| CaCO3·6H2O | Monoclinic | C12/c1(15) | 8.78 | 8.28 | 10.88 | 109.593 | 1.859 | 743.68 | This work | | |
|  |  |  | 8.84 | 8.33 | 10.98 |  | 1.807 | 765.24 | Cal. value[12] | | |
|  |  |  | 8.7316 | 8.2830 | 10.9629 | 109.043 |  |  | Exp. value[14] | | |
|  |  |  | 8.5919 | 8.2416 | 10.8094 |  |  |  | Cal. value [17] | | |
|  |  |  | 8.8053 | 8.3138 | 10.3280 |  |  | 756.02 | Cal. value [7] | | |
| CaCO3·H2O | Trigonal | P31(144) | 10.65 | 10.65 | 7.64 |  | 2.348 | 751.61 | | This work | |
|  |  |  | 10.64 | 10.64 | 7.64 |  | 2.353 | 750.22 | | Cal. value[12] | |
|  |  |  | 10.671 | 10.671 | 7.663 |  |  |  | Cal. value [17] | | |
|  |  |  | 10.554 | 10.554 | 7.564 |  |  |  | Exp. value[13] | | |

Table 3.The calculated independent elastic constants (*Cij*) (GPa), bulk modulus (*B*) (GPa), shear modulus (*G*) (GPa), Young’s modulus (*E*) (GPa), *B*/*G*, Poisson’s ratio () and Vickers hardness of calcium carbonate hydrates

|  |  |  |  |
| --- | --- | --- | --- |
| Species | CaCO3·1/2H2O | CaCO3·6H2O | CaCO3·H2O |
| *C11* | 109.28 | 48.32 | 88.97 |
| *C22* | 129.65 | 91.21 | 80.81 |
| *C33* | 83.74 | 99.93 | 72.88 |
| *C44* | 36.89 | 26.40 | 23.79 |
| *C55* | 42.38 | 32.49 | 26.11 |
| *C66* | 42.67 | 25.91 | 29.42 |
| *C12* | 36.33 | 27.06 | 21.12 |
| *C13* | 25.84 | 19.49 | 30.85 |
| *C14* |  |  | 2.44 |
| *C15* | 0.06 | -6.42 | 1.83 |
| *C16* |  |  | 28.67 |
| *C23* | 57.44 | 14.31 | -3.78 |
| *C24* |  |  | 0.25 |
| *C25* | 4.08 | 0.38 | 0.62 |
| *C26* |  |  | -1.67 |
| *C34* |  | -13.05 | 3.16 |
| *C35* |  |  | 2.36 |
| *C36* |  | -2.78 | 1.34 |
| *B* | 60.511 | 37.987 | 44.696 |
| *G* | 36.566 | 27.269 | 26.284 |
| *E* | 91.284 | 66.013 | 65.928 |
|  | 0.248 | 0.210 | 0.254 |
| *B*/*G* | 1.655 | 1.393 | 1.701 |
| *HV*Chen | 6.104 | 6.386 | 4.274 |
| *HV*Tian | 6.629 | 6.544 | 5.094 |
| *AU* | 0.454 | 0.742 | 0.155 |
| *AB* | 0.032 | 0.056 | 0.004 |
| *AG* | 0.037 | 0.059 | 0.014 |