# Unveiling the interfacial dynamic of Si/Al adsorption on calcium carbide: mechanistic insights and advanced applications

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## Content

**Table A1** Data of Figure 3 (Elemental content of calcium carbide)

| | Ca | Si | Al | Fe | S | Na | K | Mg | P | Cl | Ti | Sr |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Sample1 | 95.579 | 1.918 | 1.548 | 0.159 | 0.369 | 0.082 | 0.069 | 0.053 | 0.044 | 0.048 | 0.048 | 0.085 |
| Sample2 | 94.509 | 2.576 | 2.039 | 0.174 | 0.365 | 0.032 | 0.006 | 0.059 | 0.045 | 0.034 | 0.084 | 0.078 |

**Table A2** Data of Figure 4 (Bond length and bond population of Si and Al before and after adsorption on $CaC_2$ surface at B2 site. (a) Si before adsorption; (b) Si after adsorption; (c) Al before adsorption; (d) Al after adsorption)

| | C4-C8 | Ca12-C4 | Ca8-C8 | Ca12-C6 | Ca4-C10 | Ca4-C4 | Ca4-C8 | Ca3-C4 |
|---|---|---|---|---|---|---|---|---|
| Population | 1.67 | 0.18 | 0.18 | 0.01 | 0.01 | 0.02 | 0.02 | 0.03 |
| Length(Å) | 1.266 | 2.583 | 2.583 | 2.750 | 2.750 | 2.820 | 2.820 | 2.823 |

| | C4-C8 | Ca12-C6 | Ca4-C8 | Ca16-C8 | Ca8-C8 | C4-Si1 | C16-Si1 |
|---|---|---|---|---|---|---|---|
| Population | 1.67 | 0.02 | 0.01 | 0.15 | 0.14 | 0.64 | 0.64 |
| Length(Å) | 1.276 | 2.759 | 2.987 | 2.627 | 2.744 | 1.880 | 1.879 |

| | C4-C8 | Ca12-C4 | Ca8-C8 | Ca4-C4 | Ca3-C4 | Ca4-C8 | Ca16-C4 | Ca16-C8 | Ca3-C8 |
|---|---|---|---|---|---|---|---|---|---|
| Population | 1.67 | 0.18 | 0.18 | 0.02 | 0.03 | 0.02 | 0.02 | 0.02 | 0.03 |
| Length(Å) | 1.266 | 2.583 | 2.583 | 2.820 | 2.823 | 2.820 | 2.820 | 2.820 | 2.823 |

| | C4-C8 | Ca4-C4 | Ca12-C4 | Ca4-C8 | Ca16-C8 | C4-Al1 | C16-Al1 |
|---|---|---|---|---|---|---|---|
| Population | 1.68 | 0 | 0.01 | 0.01 | 0.13 | 0.39 | 0.39 |
| Length(Å) | 1.270 | 2.652 | 2.922 | 2.965 | 2.653 | 2.075 | 2.076 |

**Table S1** Energies of Si at different adsorption sites of $CaC_2(110)$.

| | Adsorption site | $CaC_2(110)$/(eV) | Si energy /(eV) | Total adsorbed energy /(eV) | $E_{ad}$/(eV) |
|---|---|---|---|---|---|
| Si | Ca top | -21111.79 | -170.47 | -21283.4858 | -1.2258 |
| | C1 top | | -170.47 | -21281.8441 | 0.4159 |
| | C2 top | | -170.47 | -21281.8441 | 0.4159 |
| | B1 | | -170.47 | -21283.4861 | -1.2261 |
| | B2 | | -170.47 | -21283.4861 | -1.2261 |
| | B3 | | -170.47 | -21282.6160 | -0.3560 |
| | B4 | | -170.47 | -21282.6161 | -0.3561 |
| | H1 | | -170.47 | -21281.8388 | 0.4212 |
| | H2 | | -170.47 | -21281.8388 | 0.4212 |

**Table S2** Energies of Al at different adsorption sites of $CaC_2(110)$.

| | Adsorption site | $CaC_2(110)$/(eV) | Al energy /(eV) | Total adsorbed energy /(eV) | $E_{ad}$/(eV) |
|---|---|---|---|---|---|
| Al | Ca top | -21111.79 | -109.85 | -21223.0385 | -1.3985 |
| | C1 top | | -109.85 | -21222.4481 | -0.8081 |
| | C2 top | | -109.85 | -21222.4475 | -0.8075 |
| | B1 | | -109.85 | -21223.0388 | -1.3988 |
| | B2 | | -109.85 | -21223.0395 | -1.3995 |
| | B3 | | -109.85 | -21223.0384 | -1.3984 |
| | B4 | | -109.85 | -21223.0380 | -1.3980 |
| | H1 | | -109.85 | -21222.4509 | -0.8109 |
| | H2 | | -109.85 | -21222.4502 | -0.8102 |

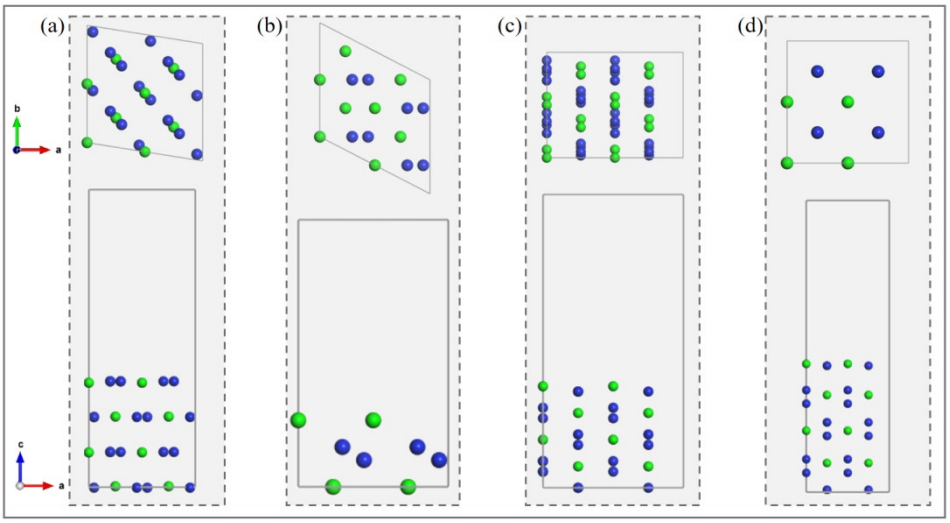


**Fig. S1** Side and top views of different crystalline surfaces of $CaC_2$ (a) (110); (b) (101); (c) (112); (d) (002). Blue and green colors represent C and Ca atoms, respectively.

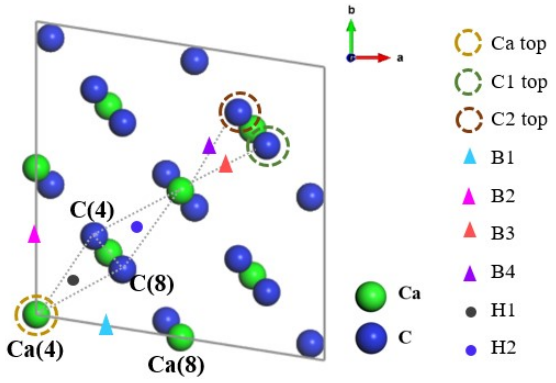


**Fig. S2** Top view schematic of possible adsorption sites on the $CaC_2$ (110) surface.

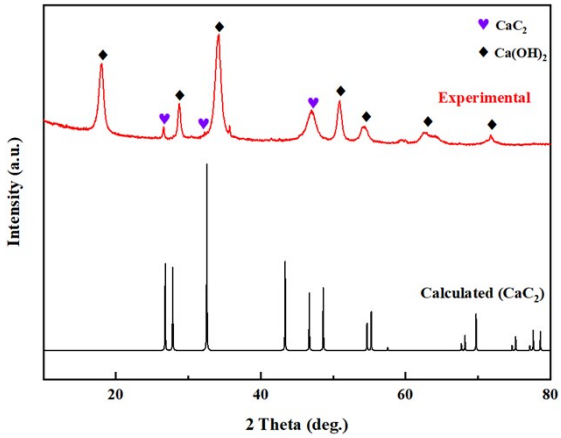


**Fig. S3** XRD image of calcium carbide.

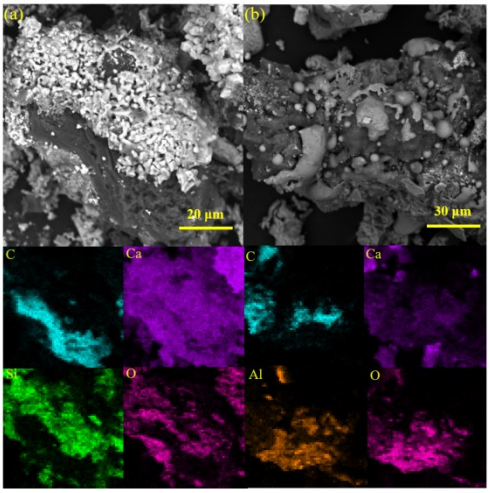


**Fig. S4** SEM-EDS images after reaction (a) after reaction of $CaC_2$ and $SiO_2$; (b) after reaction of $CaC_2$ and $Al_2O_3$.

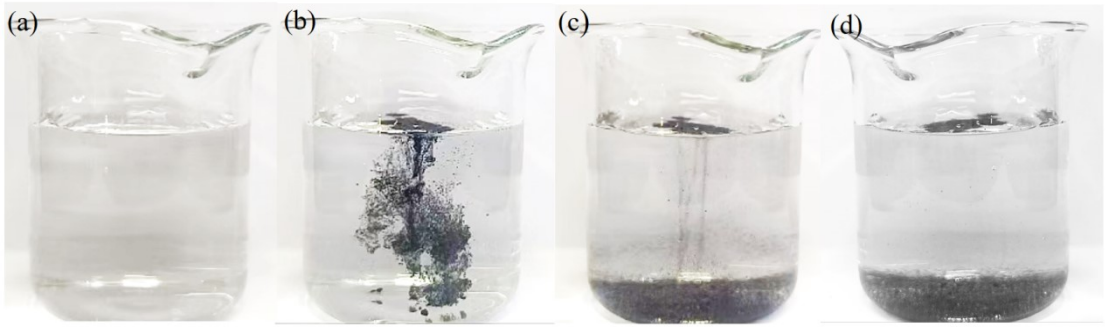


**Fig. S5** Gassing test of samples after reaction of $CaC_2$ and $SiO_2$.

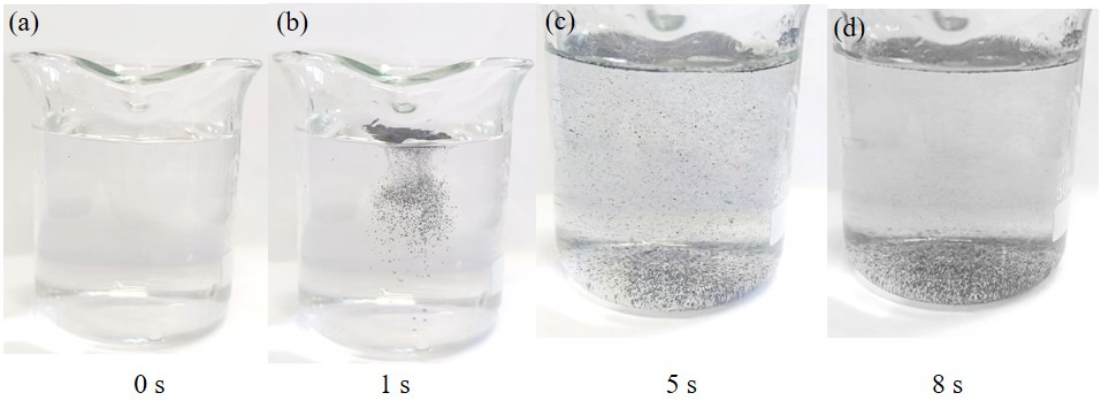


**Fig. S6** Gassing test of samples after reaction of $CaC_2$ and $Al_2O_3$.