Supporting Information for Peel Adhesion Strength between Epoxy Resin and Hydrated Silica Surfaces: A Density Functional Theory Study

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1. **Energy and adhesive force curves for the peel process of two structures shown in Figure 3b and 3c**

2. **Energy and adhesive force curves for the tensile process of two structures shown in Figure 3b and 3c**

3. **Fitting parameters and adhesion forces for each process of two structures shown in Figure 3b and 3c**

S1. Energy and adhesive force curves for the peel process of two structures shown in Figure 3b and 3c
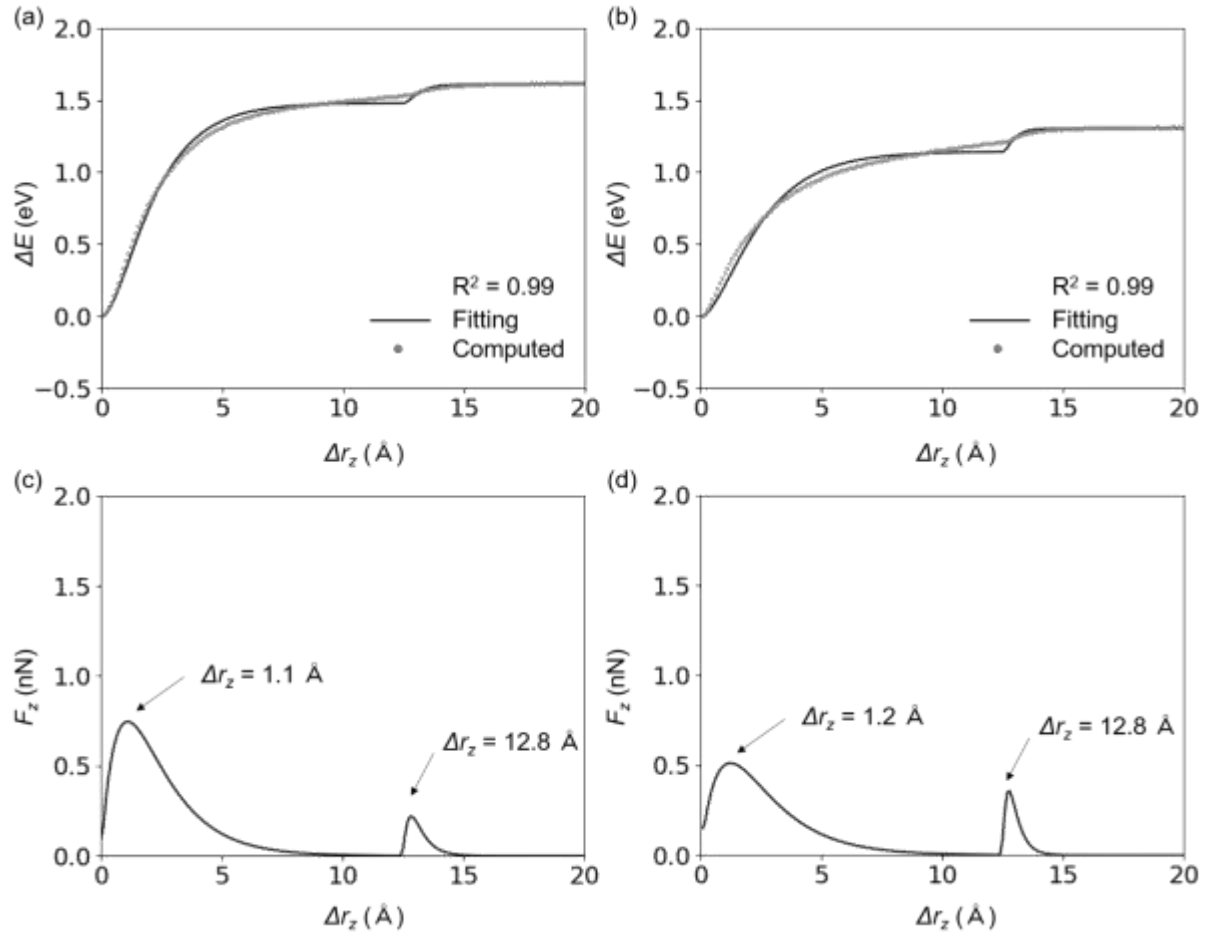
Figure S1. (a) and (b) correspond to potential energy-displacement (ΔE-Δr_z) curves for the peel process of two structures shown in Figure 3b and 3c, respectively. Each point in the gray dotted line corresponds to the value obtained from the calculation, and the black solid line corresponds to the curve obtained by fitting. (c) and (d) correspond to adhesive force-displacement (F_z - Δr_z) curves for the peel process of two structures shown in Figure 3b and 3c, respectively.

S2. Energy and adhesive force curves for the tensile process of two structures shown in Figure 3b and 3c
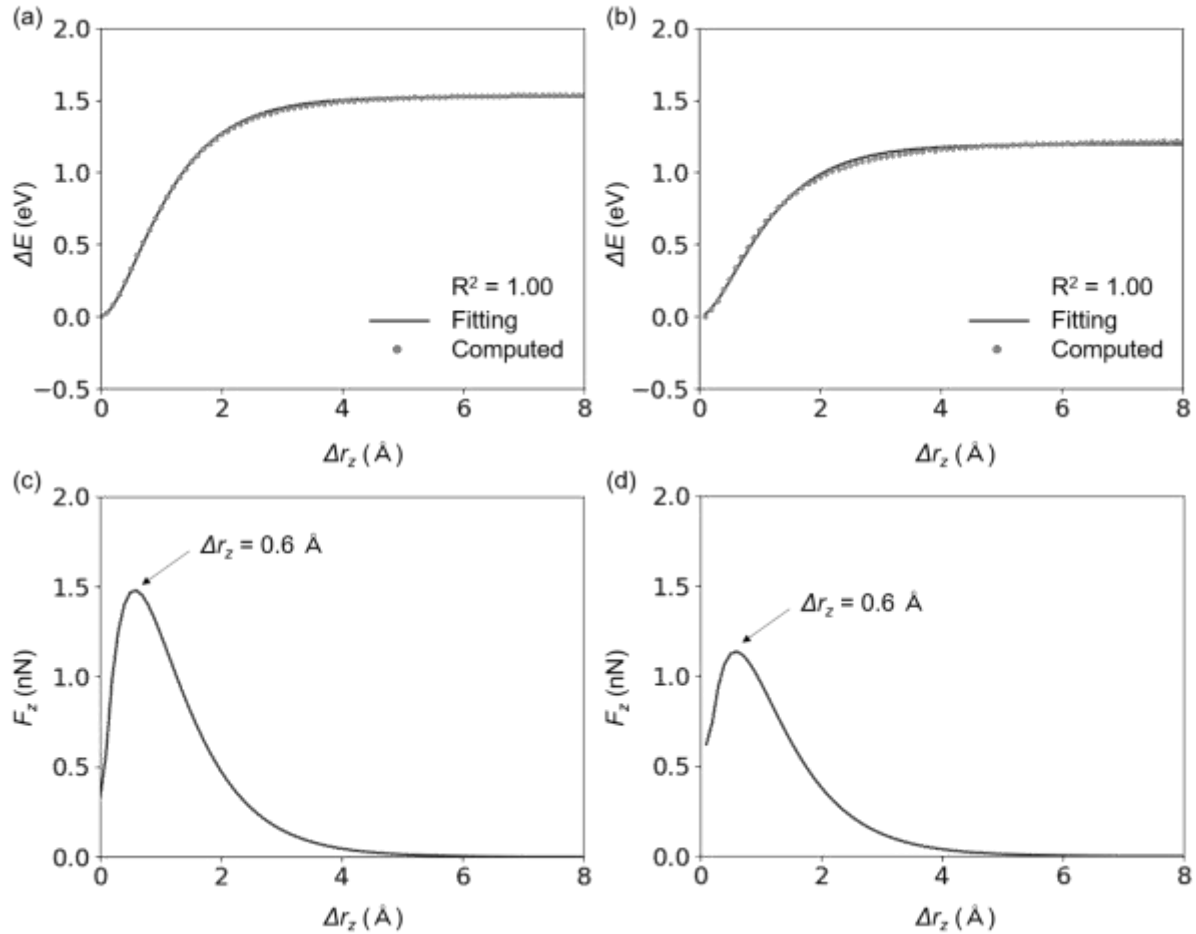
Figure S2. (a) and (b) correspond to potential energy-displacement (ΔE-Δr_z) curves for the tensile process of two structures shown in Figure 3b and 3c, respectively. Each point in the gray dotted line corresponds to the value obtained from the calculation, and the black solid line corresponds to the curve obtained by fitting. (c) and (d) correspond to adhesive force-displacement (F_z - Δr_z) curves for the tensile process of two structures shown in Figure 3b and 3c, respectively.

S3. Fitting parameters and adhesion forces for each process of two structures shown in Figure 3b and 3c

Table S1. Values of the fitting parameters (D_i and a_i), the maximum values of adhesion forces F_i, and its displacement position Δr_i for the two peel processes and the tensile process of two structures shown in Figure 3b and 3c.

Structure shown in Figure 3b				
Peel process i	D_i (eV)	a_i ($\square^{-1}$)	Δr_i ($\square$)	F_i (nN)
$i = 1$	1.48	0.63	1.1	0.75
$i = 2$	0.13	2.15	12.8	0.22
Tensile process	D (eV)	a ($\square^{-1}$)	Δr ($\square$)	F (nN)
	1.53	1.22	0.6	1.48
Structure shown in Figure 3c				
Peel process i	D_i (eV)	a_i ($\square^{-1}$)	Δr_i ($\square$)	F_i (nN)
$i = 1$	1.14	0.56	1.2	0.51
$i = 2$	0.16	2.85	12.8	0.36
Tensile process	D (eV)	a ($\square^{-1}$)	Δr ($\square$)	F (nN)
	1.19	1.19	0.6	1.14