Supplementary Material

Computational characterization of the structural and mechanical properties of nanoporous titania

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S1. Three-dimensional structures

Fig. S1 The three-dimensional structures of Model I and Model II. Gray and red represent Ti and O atom, respectively.

S2. Potential energy of structures

Fig. S2 Potential energy of bulk rutile TiO$_2$ at 300 K.
Fig. S3 Potential energy of Model I at 300 K. (a) IA. (b) IB. (c) IC. (d) ID.

Fig. S4 Potential energy of Model II at 300 K. (a) IIA. (b) IIB. (C) IIC. (d) IID. (e) IIE.

S2. Relaxed Structures
The relaxed porous structures are shown as Fig. S5 and Fig. S6.

Fig. S5 Relaxed structures of porous titania with different pore sizes.

Fig. S6 Relaxed structures of porous titania with different porosities.

S2. Structural parameters

The structural parameters (pore size, surface area, total volume, porosity and specific surface area) of the constructed models are listed in Table S1.

Table S1 Structural parameters of the constructed models.

| Model | Pore size (nm) | Surface Area (Å²) | Total volume (Å³) | Porosity (%) | Specific surface area (×10² Å⁻¹) |
|-------|----------------|-------------------|-------------------|--------------|-----------------------------------|
| IA    | 1.3            | 1444              | 39967             | 8.3          | 3.6                               |
| IB    | 2.8            | 2363              | 152875            | 8.1          | 1.5                               |
| IC    | 3.4            | 3072              | 252794            | 8.3          | 1.2                               |
| ID    | 5.1            | 4395              | 527570            | 8.0          | 0.8                               |
| IIA   | 2.8            | 2363              | 152875            | 8.1          | 1.5                               |
S3. Parameters of three force fields

Table S2. Parameters of the Matsui-Akaogi (MA) force fields

| i-j  | $A_{ij}$ (kcal/mol) | $\rho_{ij}$ (Å) | $C_{ij}$ (kcal/mol Å$^6$) |
|------|---------------------|-----------------|---------------------------|
| Ti-Ti| 717895.18           | 0.154           | 121.037                   |
| Ti-O | 391184.85           | 0.194           | 290.489                   |
| O-O  | 271810.46           | 0.234           | 697.175                   |

Atomic charges: $q$(Ti) = 2.196 (e), $q$(O) = -1.098 (e)

Table S3. Parameters of the modified-MA force fields

| i-j  | $A_{ij}$ (kcal/mol) | $\rho_{ij}$ (Å) | $\sigma_{ij}$ (Å) | $C_{ij}$ (kcal/mol Å$^6$) | $D_{ij}$ (kcal/mol Å$^8$) |
|------|---------------------|-----------------|-----------------|---------------------------|---------------------------|
| Ti-Ti| 415086.9482         | 0.25            | 0               | 18448.30881               | 11530.193                |
| Ti-O | 68339.20028         | 0.248213237     | 0               | 334.6753822               | 63.41606153              |
| O-O  | 51053.61919         | 0.343644974     | 0               | 4440.969138               | 2444.400917              |

Atomic charges: $q$(Ti) = 2.196 (e), $q$(O) = -1.098 (e)

Table S4. Parameters of the MS-Q force fields

| i-j  | $A_{ij}$ (kcal/mol) | $B_{ij}$ (Å$^{-1}$) | $r_0$ (Å) |
|------|---------------------|---------------------|-----------|
| Ti-Ti| 0.130784443         | 1.5543              | 4.18784   |
| Ti-O | 23.70490766         | 3.640737            | 1.88265   |
| O-O  | 0.971234278         | 1.1861              | 3.70366   |

Atomic charges: $q$(Ti) = 1.151 (e), $q$(O) = -0.576 (e)

S4. Elastic property

Bulk modulus ($K$), shear modulus ($G$) and Young’s modulus ($E$) and Poisson ratio ($\eta$) were evaluated from the computed elastic constants with the Voigt-Reuss-Hill method:

$$K = \frac{1}{2} (K_V + K_S) \quad (S1)$$

$$G = \frac{1}{2} (G_V + G_S) \quad (S2)$$
where the subscript of \( V \) and \( R \) respectively represent the elastic moduli of Voigt theory and Reuss theory.

\[
E = \frac{9KG}{3K + G} \quad \text{(S3)}
\]

\[
\eta = \frac{3K - 2G}{2(3K + G)} \quad \text{(S4)}
\]

\[
K_V = \frac{1}{9} [C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] \quad \text{(S5)}
\]

\[
G_V = \frac{1}{15} [C_{11} + C_{12} + C_{33} + 2(C_{12} + C_{55} + C_{66}) - (C_{12} + C_{13} + C_{23})] \quad \text{(S6)}
\]

\[
K_R = [C_{11}(C_{22} + C_{33} - 2C_{23}) + C_{22}(C_{33} - 2C_{13}) - 2C_{33}C_{12}
+ C_{12}(2C_{23} - C_{12}) + C_{13}(2C_{12} - C_{13}) + C_{23}(2C_{13} - C_{23})]^{-1} \quad \text{(S7)}
\]

\[
G_R = 15 \{4[C_{11}(C_{22} + C_{33} + C_{23}) + C_{22}(C_{33} + C_{13}) + C_{33}C_{12}
- C_{12}(C_{23} + C_{12}) - C_{13}(C_{12} + C_{13}) - C_{23}(C_{13} + C_{23})]/C_X
+ 3\left(\frac{1}{C_{44}} + \frac{1}{C_{55}} + \frac{1}{C_{66}}\right)\}^{-1} \quad \text{(S8)}
\]

\[
C_X = C_{13}(C_{12}C_{23} - C_{13}C_{22}) + C_{23}(C_{12}C_{13} - C_{11}C_{23})
+ C_{33}(C_{11}C_{22} - C_{12}C_{12}) \quad \text{(S9)}
\]