

Supporting Information

Title:

**Effective Functionalization of Disordered Oxide Lattices
on Iron Particle Surfaces Using Mechanochemical Reactions**

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Figure S1

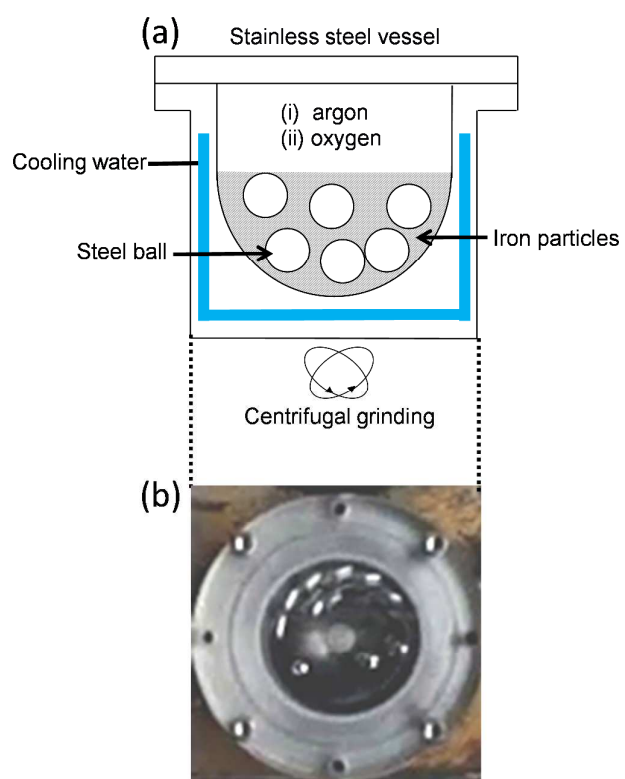
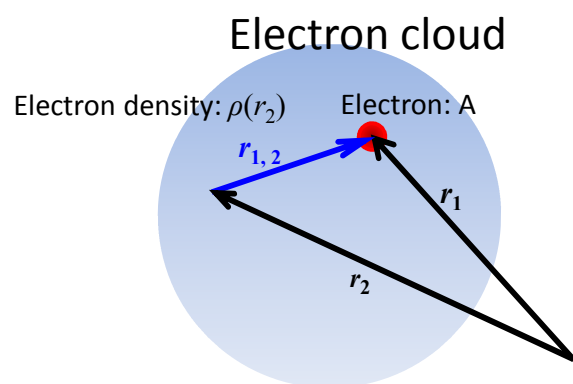


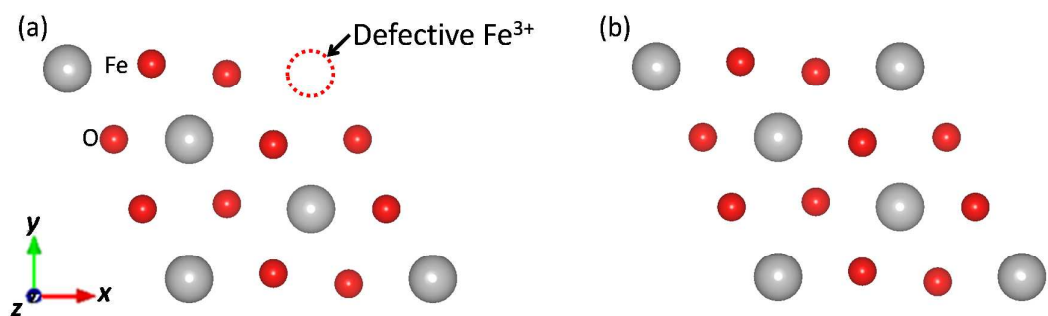
Figure S1. (a) Set-up for the mechanochemical reaction, and (b) photograph of the top view of the equipment during the milling.

Scheme S1



Scheme S1. Relationship of the r_1 , r_2 and $r_{1,2}$ at equation(8).

Scheme S2



Scheme S2. Model clusters by molecular orbital calculations of (a) α -Fe₂O₃ surface with the disordered lattice induced by defective Fe³⁺ ion, and (b) Fe₂O₃ crystal with ordered lattice (O atom: red, Fe atom: gray).

Figure S2

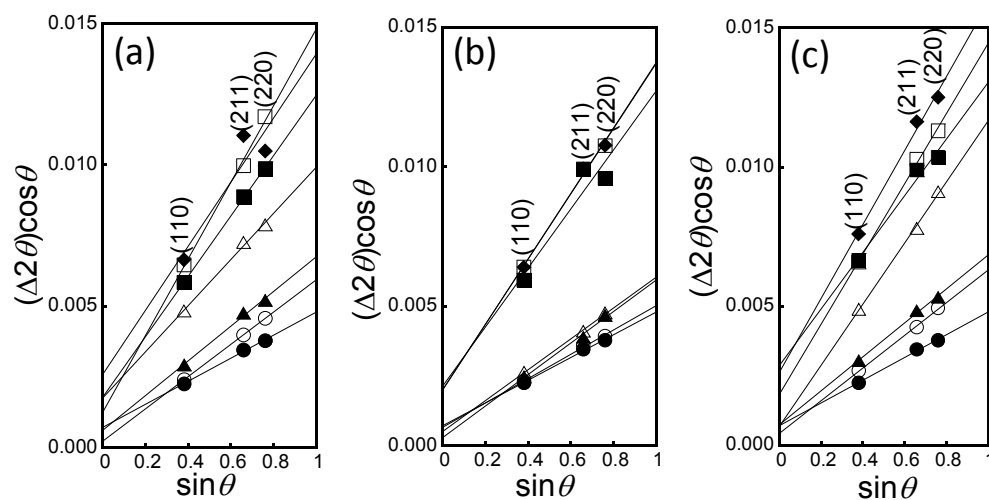


Figure S2. Williamson-Hall plots of the iron particles milled by the force of (a) 149 mN, (b) 256 mN and (c) 439 mN at the time of 0 h, 0.5 h, 2 h, 8 h, 16 h, 24 h and 32 h, which are represented by ●, ○, ▲, △, ■, □, ◆, respectively, in the plots, which were calculated from the XRD patterns of the Figure 2 in the text.

Figure S3

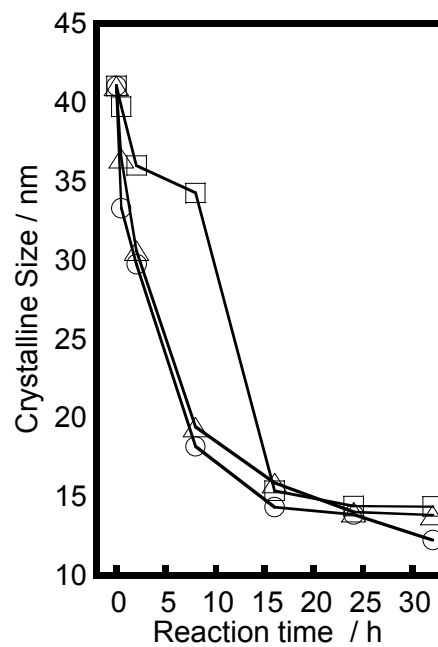


Figure S3. Crystallite sizes with the reaction time by the different milling forces of (○) 153 mN, (□) 283 mN and (△) 439 mN, which are calculated by the Scherer's equation.

Figure S4

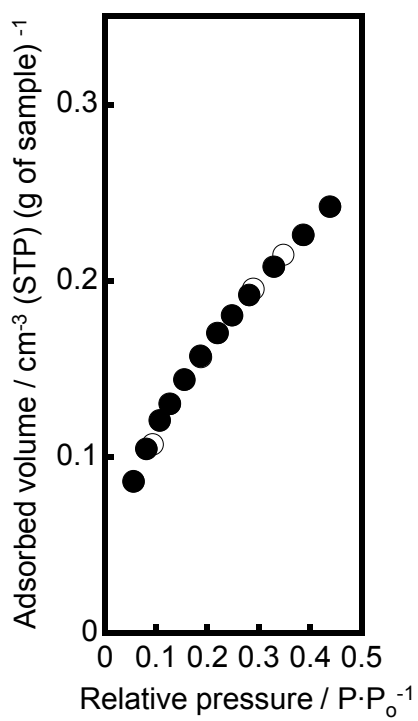


Figure S4. Krypton adsorption (closed circles) and desorption (open circles) isotherms of the bare ion particles before the milling.

Figure S5

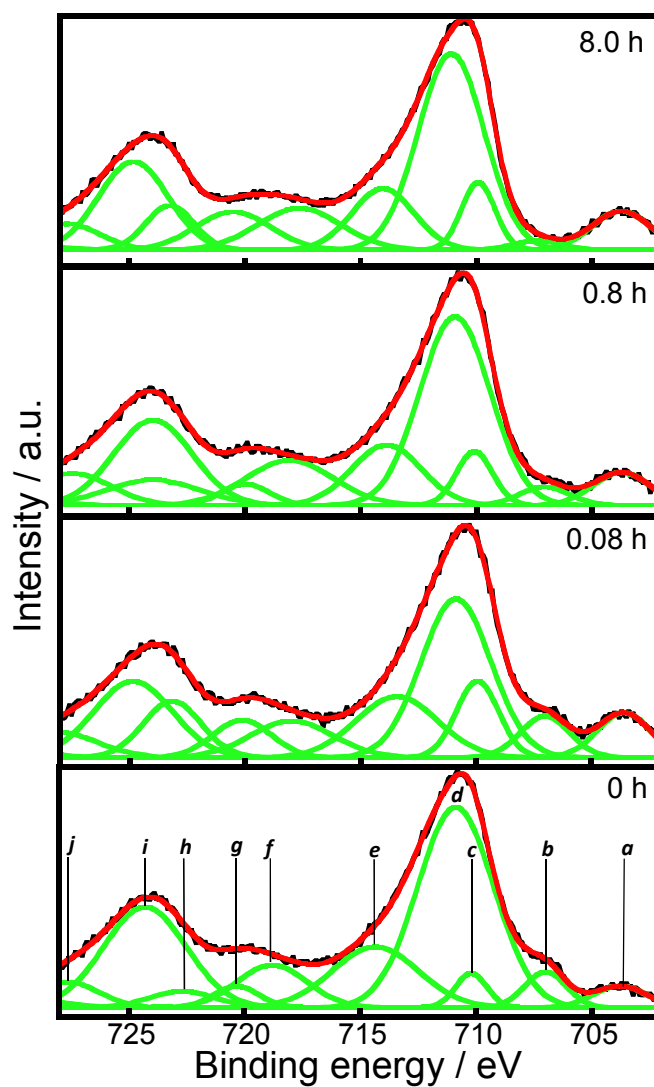


Figure S5. Deconvolution results of XPS spectra from Fe 2*p* of the milled iron particles reacted with oxygen molecules at the different time, which were adequately separated into ten peaks (*a*: In 3*p*_{1/2}, *b*: Fe⁰ 2*p*_{3/2}, *c*: Fe²⁺ 2*p*_{3/2} (Fe₃O₄), *d*: Fe³⁺ 2*p*_{3/2} (a-Fe₂O₃), *e*: Sat. Fe²⁺ 2*p*_{3/2} (Fe₃O₄), *f*: Sat. Fe³⁺ 2*p*_{3/2} (a-Fe₂O₃), *g*: Fe⁰ 2*p*_{1/2}, *h*: Fe²⁺ 2*p*_{1/2} (Fe₃O₄), *i*: Fe³⁺ 2*p*_{1/2} (a-Fe₂O₃), *j*: Sat. Fe²⁺ 2*p*_{1/2} (Fe₃O₄)).