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SUPPLEMENTARY MATERIAL TO

Molecular docking's pioneering role in materials science. Metal ion site-preference in fluorapatite

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METHODOLOGY

SM1. DFT calculations

The wb97xd method, a long-range corrected hybrid density functional, was employed for the calculations, providing the satisfactory accuracy for thermochemistry, kinetics, covalent systems, and both short-range and long-range non-covalent interactions. All density functional theory (DFT) calculations were executed using the Gaussian09 program. To ensure the generation of reliable interaction strength data, four distinct basis sets (def2-TZVP, jorge-TZP, x2c-TZVPall, and dgauss-DZVP basis set) were applied to the model system, consisting solely of a Mn^{2+} ion and a phosphate group. The distance between the metal ion and the nearest oxygen atom of the phosphate group was systematically varied during the calculations, from 2.0 to 3.0 Å. Importantly, this variation was performed in a manner that maintained the linear orientation of the interacting atoms, with the phosphorus atom forming a fixed angle (M···O-P angle fixed at 180°).

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RESULTS AND DISCUSSION

SM2. Analysis of crystal structures

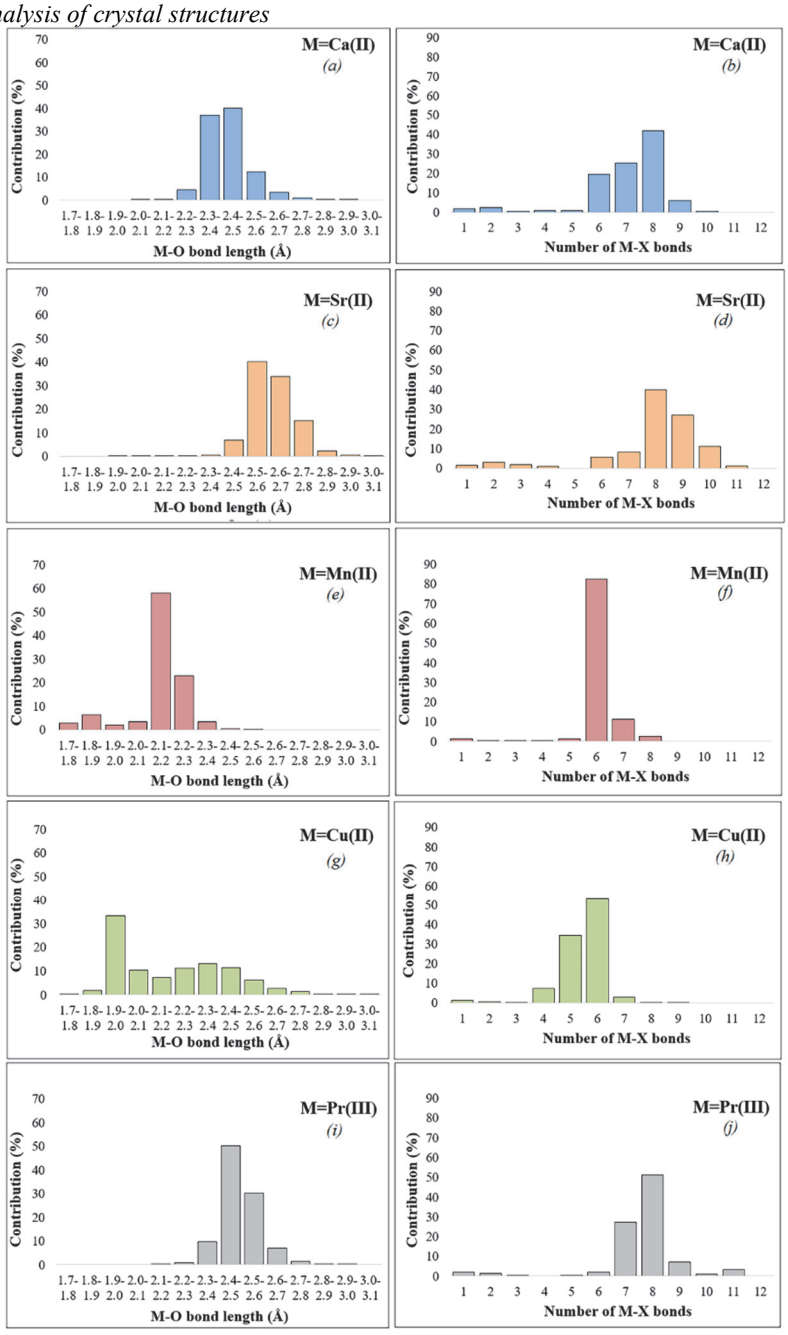

Fig. S-1. Geometrical parameters for M-O bonds (M = Ca^{2+}, Sr^{2+}, Mn^{2+}, Cu^{2+}, and Pr^{3+}) extracted from crystal structures of small molecules, archived in the CSD.

SM3. DFT calculations

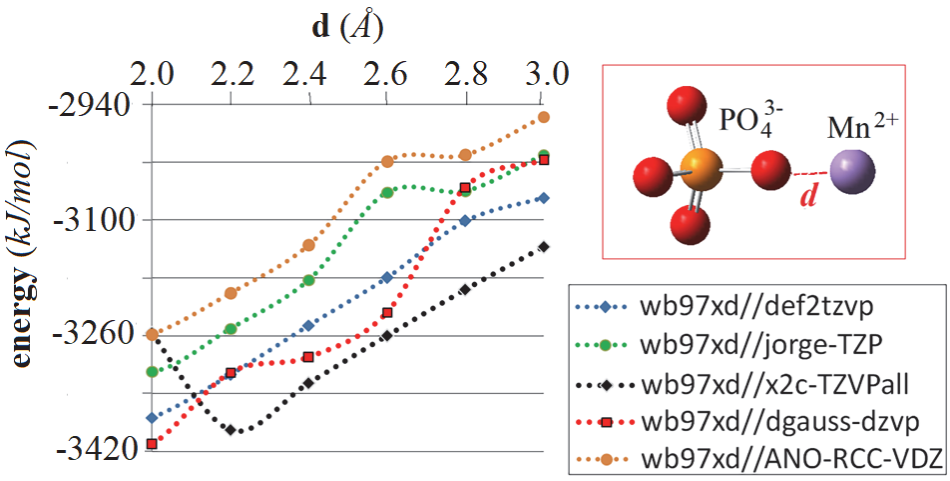

Fig. S-2. Results of DFT calculations for evaluation of the interaction energies between the phosphate group and the metal M ion (M = Ca^{2+}, Sr^{2+}, Mn^{2+}, Cu^{2+} or Pr^{3+} ion). Parameter *d* represents the distance between the metal ion and the nearest oxygen O atom, with the linear geometry of the interacting atoms and phosphorus atom (M···O-P angle is equal to 180°).

SM4. Molecular docking study

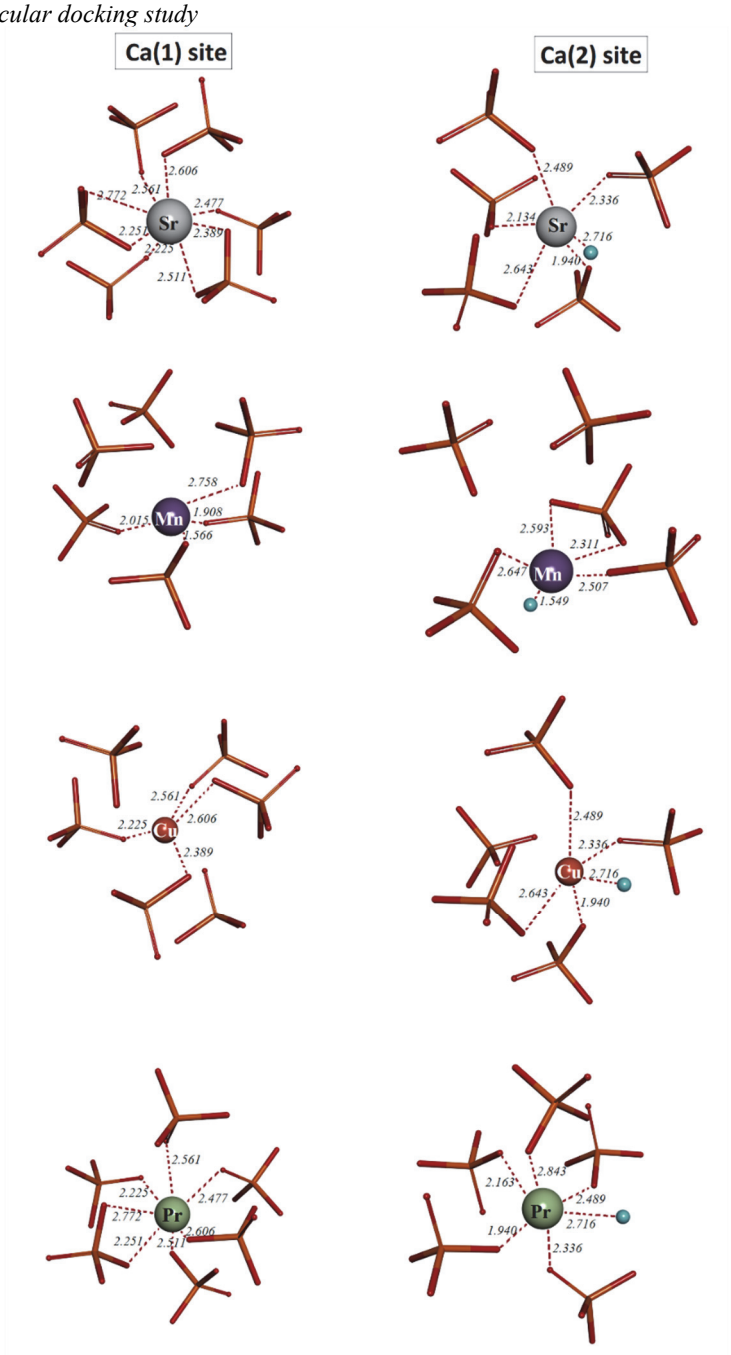

Fig. S-3. Interactions of metal ions (Sr^{2+}, Mn^{2+}, Cu^{2+}, and Pr^{3+}) in site 1 (left) and site 2 (right), obtained by the docking study.