Supplemental Information for:

Unveiling mechanism of tuning elemental distribution in high entropy alloys and its effect on thermal stability

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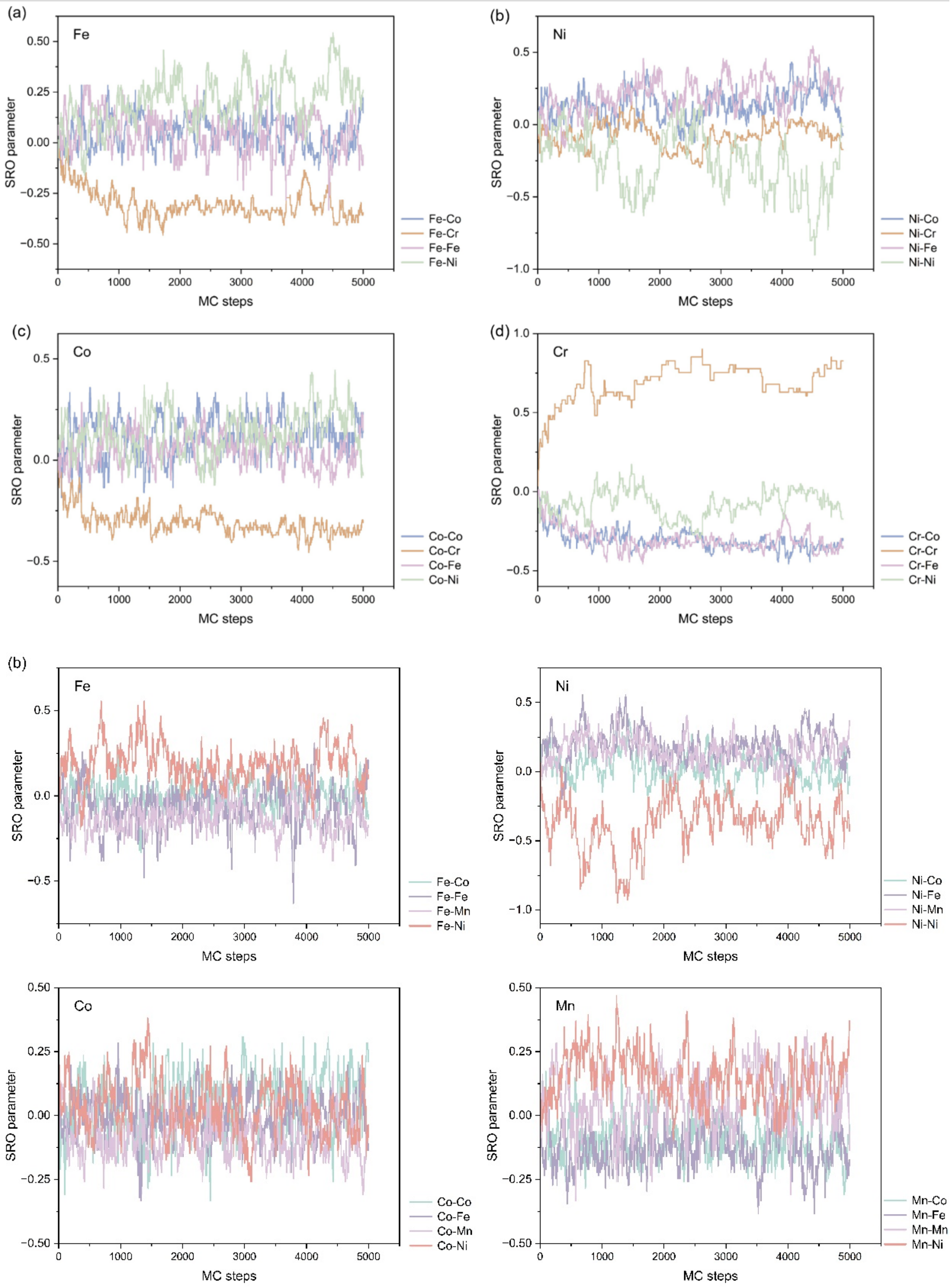

Fig. S1 1NN chemical SRO parameter of CoFeNiCr and CoFeNiMn HEA. (a) CoFeNiCr HEA; (b) CoFeNiMn HEA.

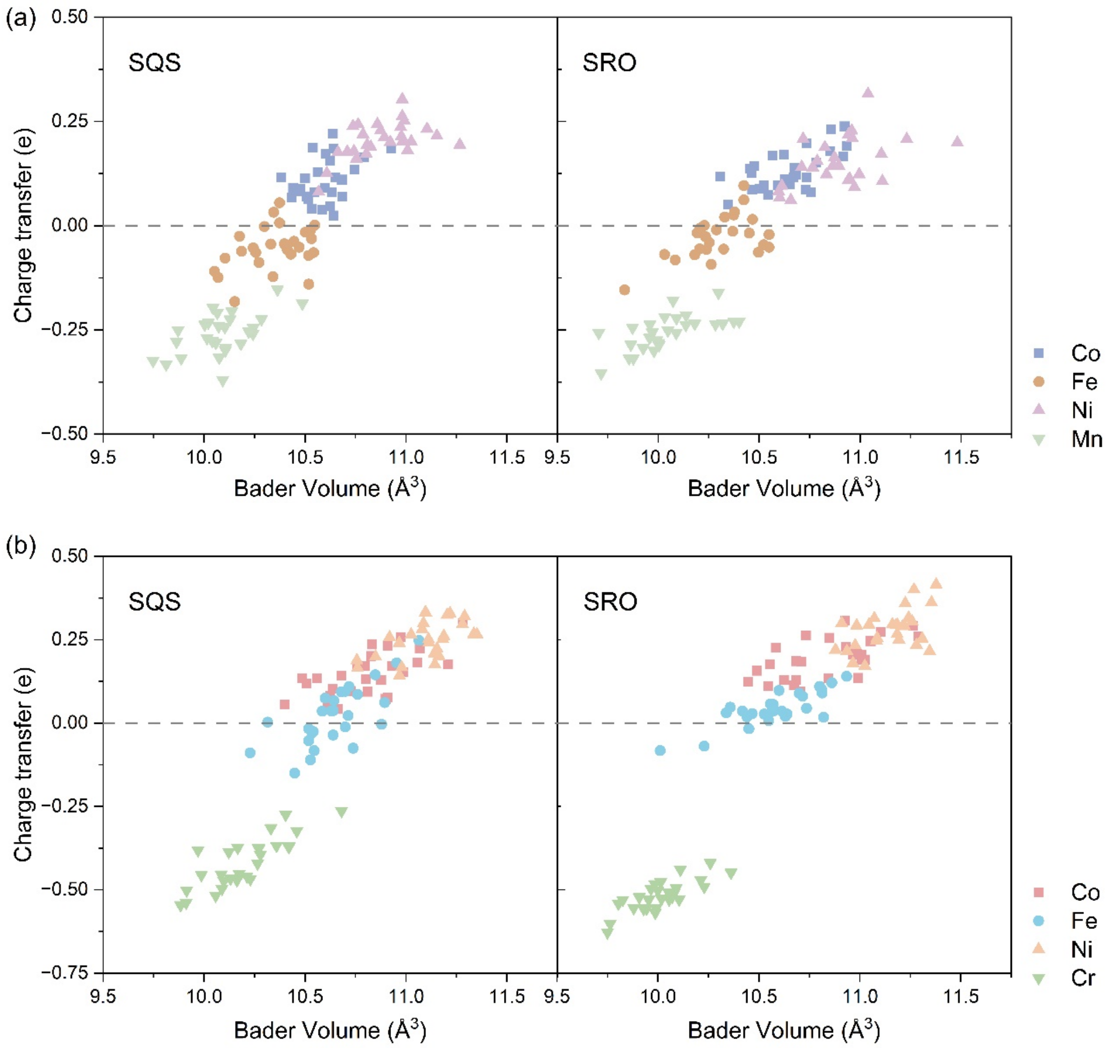

Fig. S2 Correlation between Charge transfer and Bader Volume. (a) CoFeNiMn; (b) CoFeNiCr.

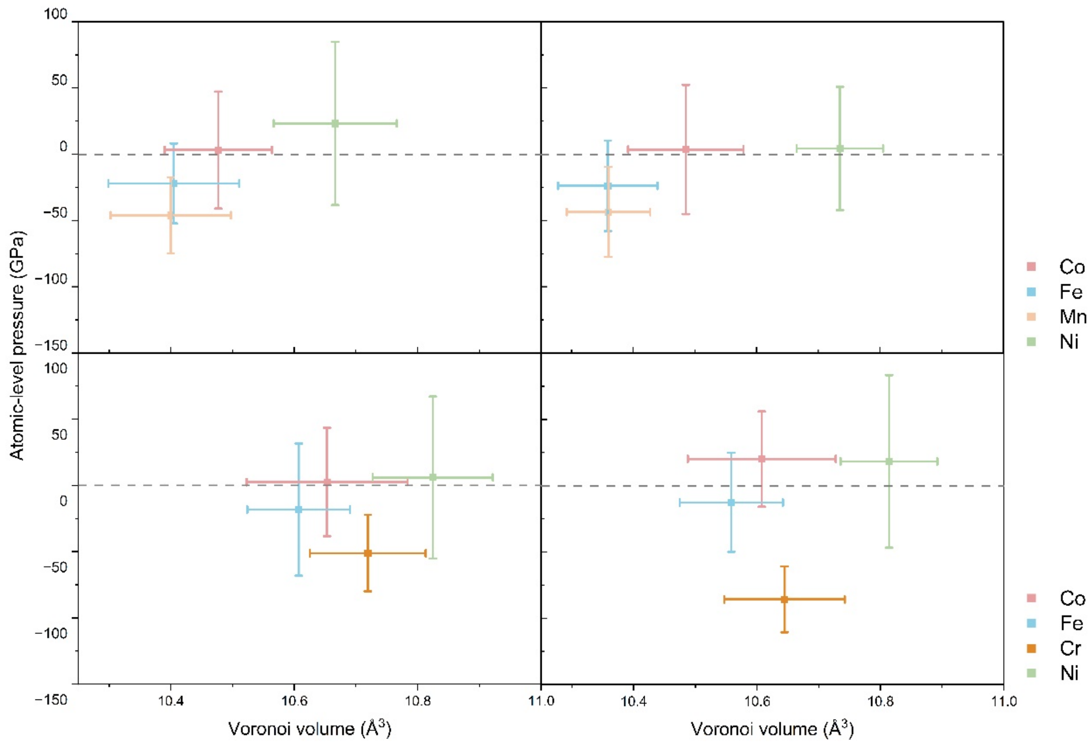

Fig. S3 Correlation between Ave. charge transfer and Ave. Bader Volume. (a) CoFeNiMn; (b) CoFeNiCr.

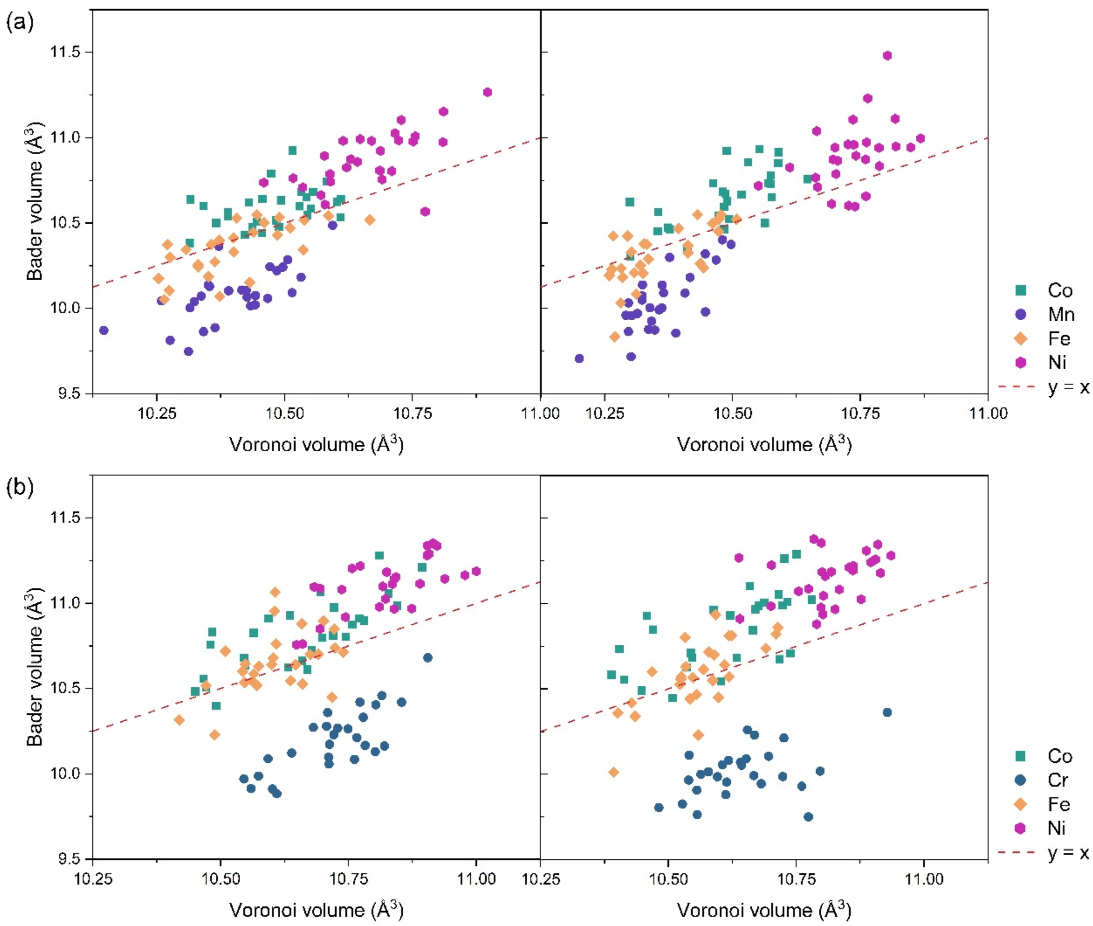

Fig. S4 Correlation between Voronoi volume and Bader Volume. (a) CoFeNiMn; (b) CoFeNiCr. Left corresponds to SQS structures, and right corresponds to SRO structures. The red dashed line represents the asymptote $y = x$.

Strain-Stress calculations

Elastic constants are crucial physical properties that characterize a material's ability to deform under small stresses. These constants can be determined by describing a physical quantity as a fourth-order tensor C_{ijkl}. This tensor establishes the relationship between the second-order stress tensor σ_{ij} and the second-order strain tensor e_{kl}, following the generalized Hooke's Law:

$$\sigma_{ij} = C_{ijkl} e_{kl}$$

The above formula can be simplified using the Voigt-Reuss-Hill (VRH) averaging method[1]. In the calculations for Voigt and Reuss averages, the Poisson's ratio is neglected. This is because Voigt average assumes uniform strain in each phase, while Reuss average assumes uniform stress in each phase. This simplification is represented by a square 6×6 matrix C_{mn} to denote the fourth-order tensor C_{ijkl}, and the simplified formula becomes

$$\sigma_i = C_{ij} e_j$$

The lattice vectors a_{ij}' of a crystal affected by strain can be obtained through the relationship between the original lattice vectors a_{ij}^0 and the strain tensor e_{ij}. We relax the system in the x and y directions while subjecting 1% change in the z direction.

Reference

1. R. Hill, *Proc. Phys. Soc. London, Sect. A*, 1952, **65**, 349.