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Author Correction: Physics guided deep learning for generative design of crystal materials with symmetry constraints

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Correction to: *npj Computational Materials* https://doi.org/10.1038/s41524-023-00987-9, published online 18 March 2023

The original version of this Article contained typos in both the PDF and the HTML versions.

In the fourth and fifth sentences of the first paragraph of the 'Case study of three example stable materials' section of the Results, the incorrect expression "β = β" has been replaced by "α = β".

The third note of Equation 1 incorrectly read "(c) P = (a, b, c, β, β, γ) ∈ R are six lattice parameters that define three lengths and three angles of the unit cell;" The correct version states '(a, b, c, α, β, γ)' in replace of (a, b, c, β, β, γ).

The Figure caption of Figure 5d incorrectly read "Inter- and intra-atom distance matrices (H_{inter} and H_{inter}) are calculated from three sets of base atom sites for both real and fake materials." The correct version states 'H_{intra} and H_{inter}' in replace of 'H_{inter} and H_{inter}'.

The first sentence after Equation (5) incorrectly read "where Linter constrains the distance in H_{intra} which describes inter-atom distance matrices.". The correct version states 'H_{inter}' in replace of 'H_{intra}'.

The third sentence after Equation (5) incorrectly read "S_{intra} are atom radius sum corresponding to each pair of atoms in H_{intra} and ϕ_{inter}^{upper} and ϕ_{inter}^{lower} are control weights for upper and lower bound of inter-atom distance, respectively." In the correct version, 'S_{intra}'and 'H_{intra}' have been replaced by 'S_{inter}'and 'H_{inter}', respectively.

The first sentence of the fifth paragraph of "Implementation details" section incorrectly read "Atom Distance Matrices Given three sets of base atom sites (B^0, B^1, B^2), we calculate the atom distance matrices H_{inter} and H_{inter} as shown in sub-figure (d) of Fig. 5." The correct version states 'H_{inter} and H_{intra}' in replace of 'H_{inter} and H_{inter}'.

The third sentence of the fifth paragraph of "Implementation details" section incorrectly read "Then we select three atoms belonging to the same element to form a set of three atom sites for three elements and calculate pair-wise same atom distance matrix and again return only values in upper triangle of corresponding distance matrix termed by H_{inter}." The correct version states 'H_{intra}' in replace of 'H_{inter}'.

The last sentence of the fifth paragraph of "Implementation details" section incorrectly read "The final shape of H_{inter} and H_{inter} both is 3×3." The correct version states 'H_{intra} and H_{inter}' in replace of 'H_{inter} and H_{inter}'.

The sentence before Equation (8) incorrectly read "Fractional coordinates can be converted to Cartesian coordinates $[x, y, y]^T$." The correct version states '$[x, y, z]^T$' in replace of '$[x, y, y]^T$'.

The original version of this Article contained typographical errors in Equation (9).

The correct version of Equation (9) is:

$$A = \begin{bmatrix} a & b\cos\boldsymbol{\gamma} & c\cos\boldsymbol{\beta} \\ 0 & b\sin\boldsymbol{\gamma} & c\frac{\cos\boldsymbol{\alpha}-\cos\boldsymbol{\beta}\cos\boldsymbol{\gamma}}{\sin\boldsymbol{\gamma}} \\ 0 & 0 & \frac{V}{ab\sin\boldsymbol{\gamma}} \end{bmatrix},$$

Where $V = abc\sqrt{1-\cos^2\boldsymbol{\alpha}-\cos^2\boldsymbol{\beta}-\cos^2\boldsymbol{\gamma}+2\cos\boldsymbol{\alpha}\cos\boldsymbol{\beta}\cos\boldsymbol{\gamma}}$ is the volume of the unit cell.

Which replaces the previous incorrect version:

$$A = \begin{bmatrix} a & b\cos\boldsymbol{\gamma} & c\cos\boldsymbol{\beta} \\ 0 & b\sin\boldsymbol{\gamma} & c\frac{\cos\boldsymbol{\beta}-\cos\boldsymbol{\beta}\cos\boldsymbol{\gamma}}{\sin\boldsymbol{\gamma}} \\ 0 & 0 & \frac{V}{ab\sin\boldsymbol{\gamma}} \end{bmatrix},$$

Where $V = abc\sqrt{1-\cos^2\boldsymbol{\beta}-\cos^2\beta-\cos^2\gamma+2\cos\boldsymbol{\beta}\cos\beta\cos\gamma}$ is the volume of the unit cell.

The above changes have been made in the PDF version of the Article.

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