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## UC Berkeley Previously Published Works

### Title

Correction to Benchmarking Coordination Number Prediction Algorithms on Inorganic Crystal Structures

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Page 1593. Equation 14 should read

$$w_{ij}^{dc} = \begin{cases} 1, & d_{ij} \leq d_{low}^{cut} \\ \cos \left( \frac{\pi(d_{ij} - d_{low}^{cut})}{d_{high}^{cut} - d_{low}^{cut}} + 1 \right) / 2, & d_{ij} < d_{high}^{cut} \\ 0, & d_{ij} \geq d_{high}^{cut} \end{cases}$$

$$d_{low}^{cut} = r_i + r_j + \delta_{low}^{cut}$$

$$d_{high}^{cut} = r_i + r_j + \delta_{high}^{cut}$$

(14)

Equation 15 should read

$$w_{ij}^{en} = 1 + \delta^{en} \sqrt{\frac{|X_i - X_j|}{3.3}}$$

(15)

Equation 16 should read

$$w_{ij} = \frac{w_{ij}^{Vor} \times w_{ij}^{en}}{\max\{w_{ij}^{Vor} \times w_{ij}^{en}; j = 1 \dots n\}} \times w_{ij}^{dc}$$

(16)

The corrections are typographical errors only and do not alter the results or analysis in the original manuscript.