
Corrigendum to Eng. Life Sci. 2008, 8, 507–522: “Exploiting the Link between Protein Rigidity and Thermostability for Data-Driven Protein Engineering” by S. Radestock and H. Gohlke

In chapter 2.2.4.2, the cluster configuration entropy has been erroneously defined as a function of the probability that a vertex, i.e., atom, is part of a cluster of size s , i.e., s -cluster. This is the original definition given by Andraud et al. as a morphological descriptor for heterogeneous materials [1]. However, in our work a modified version was used. The correct definition should read: “Cluster configuration entropy is defined as a function of the probability that a vertex, i.e., atom, is part of a cluster of size s^2 , i.e., s^2 -cluster.” Eq. (2) of the paper should thus be replaced by Eq. (2’):

$$w_s = \frac{s^2 n_s}{\sum_s s^2 n_s}. \quad (2')$$

The usage of s^2 instead of s does not affect the meaning of the cluster configuration entropy in general. Our modification

using s^2 , however, is more sensitive to the transition between the flexible state of the network and a state, where a large cluster *starts* to dominate the system. Thus, our modification is particularly useful to detect the beginning of the rigidification of the network, whereas the formulation given by Andraud et al. is useful to detect when the whole network becomes rigid. As shown in the article, our modification is suitable for identifying the relevant phase transition during the thermal unfolding simulation that is related to the folded-unfolded transition, where a folding core breaks down, and, hence, for the characterization of unfolding nuclei or “weak spots” of the protein structure.

We apologize for this mistake. We note that this correction does not affect any results or conclusions of the study.

- [1] C. Andraud, A. Beghdadi, J. Lafait, Entropic analysis of random morphologies, *Physica A* **1994**, 207 (1–3), 208–212.