



Authors' reply

Kinam Park & D. Robert Lu

To cite this article: Kinam Park & D. Robert Lu (1991) Authors' reply, Journal of Biomaterials Science, Polymer Edition, 2:4, 321-322, DOI: [10.1163/156856291X00214](https://doi.org/10.1163/156856291X00214)

To link to this article: <https://doi.org/10.1163/156856291X00214>



Published online: 02 Apr 2012.



Submit your article to this journal [↗](#)



Article views: 9



View related articles [↗](#)

Authors' reply

Concern was raised as to whether the results of our recent report [1] on the calculation of protein-surface interaction energy were consistent with the mathematical model presented. Pitt and Weaver have pointed out that the interaction energy should not be positive in the absence of electrostatic interactions regardless of the orientation of a protein on the surface, if the closest contact distance between the protein and the surface is the sum of the van der Waals radii of the two contacting atoms. We cannot agree more.

It should be noted, however, that the closest contact distance used in our calculation was set to be 90% of the sum of the van der Waals radii. The van der Waals radii used in our calculation were 1.00, 1.35, 1.35, 1.60, and 1.85 Å, for H, N, O, C, and S, respectively [2]. These values are comparable with those found in other references [3-6]. When the interaction energies were calculated without a multiplication factor of 0.9, no positive interaction energies were observed. Thus, the positive interaction energies observed with some protein orientations were due to a closest contact distance smaller than the sum of the van der Waals radii by 10%. This was explained to Pitt when he inquired of Lu about the meaning of 'brought to just contact'.

When only a small number of atoms are in close proximity to the surface as in Fig. 5 of our paper [1], the repulsive energy arising from the contact of the two closest atoms dominates over the attractive energies of other atom pairs. However, when a large number of atoms are in the vicinity of the surface as in Fig. 4 of our paper [1], the attractive interactions arising from the majority of atom pairs dominate over the repulsive interaction. Thus, the repulsive energy occurs when a protein molecule adsorbs in an end-on orientation rather than in a side-on orientation as described in the paper.

One could ask why we used a multiplication factor of 0.9 in the calculation of the closest contact distance. Initially, the factor of 0.9 was adapted after Coghlan and Fraga [2], who developed a semi-empirical formulation used in our study for the calculation of the protein-surface interaction energy. When we calculated the average interaction energy of 1633 different orientations of a protein on the surface as a function of the contact distance, we found that the minimum average interaction energy was maintained while the contact distance varied from 90% to 110% of the sum of the van der Waals radii. In addition, Hopfinger has pointed out that there is no single set of van der Waals radii which can be assigned to a set of atoms so that the correct contact distance is reproduced for every pairwise interaction [3]. Thus, it was natural for us to adapt the values of van der Waals radii and a multiplication factor of 0.9 from the program of Coghlan and Fraga [2].

In conclusion, we agree with Pitt and Weaver that there should not be a positive interaction energy if the closest contact distance is the sum of the van der Waals radii of the two atoms in contact. We would like to point out, however, that a positive interaction energy can result in our model when the closest contact distance is 10%

less than the sum of the van der Waals radii, and that the results presented in our paper were consistent with the mathematical model presented.

KINAM PARK and D. ROBERT LU

*Purdue University
School of Pharmacy
West Lafayette, IN 47907, USA*

REFERENCES

1. D. R. Lu and K. Park, *J. Biomater. Sci. Polymer Edn* **1**, 243 (1990).
2. B. Coghland and S. Fraga, *Computer Phys. Commun.* **36**, 391 (1985).
3. A. J. Hopfinger, *Conformational Properties of Macromolecules*, Ch. 2. Academic Press, New York (1973).
4. J. A. Dean, *Lange's Handbook of Chemistry*, 13th edn, Section 3. McGraw-Hill, New York (1985).
5. R. C. Weast, *CRC Handbook of Chemistry and Physics*, 66th edn, pD-188. CRC Press, Boca Raton, FL (1985).
6. J. N. Israelachvili, *Intermolecular and Surface Forces*, Ch. 7. Academic Press, London (1985).