

Michel, Copley, and Neumann Reply: The authors of the Comment [1] point out the sensitivity of the calculated physical properties of solid C_{60} to details of the intermolecular potential. We agree with their principal statement that the choice of interaction sites at atomic positions favors the $l=l'=10$ term in the interaction matrix. We have been well aware of this fact, and indeed referred in our Letter [2] to an extension of the theory to molecular models which include interaction sites at the centers of single and double bonds. The extended theory [3] also provides for a distribution of electric charges at specific symmetry sites of the molecule [4]. Inclusion of double bonds as interaction sites is found to increase the relative importance of the $l=6$ mode in contributing to the interaction potential and to the crystal-field term. On the other hand, single-bond interaction sites again favor the $l=10$ mode. Most important is the fact [3] that double-bond centers give a contribution to the crystal field for $l=6$ and $l=12$ which is opposite in sign to the contributions due to atoms and single bonds. These results can be checked for the case that $l=6$ by inspection of Fig. 1 in Ref. [1].

In general the orientational order parameter is a linear combination of rotator functions belonging to the manifolds $l=10$, $l=6$, and to a lesser extent higher values of l . The essential point is that this linear combination still has T_{2g} symmetry. Therefore, as we have already stated [2], the structure of the theory remains unchanged.

There is a very subtle interplay among interaction sites on atoms, and at the centers of double and single bonds, in determining the intermolecular potential and the crystal field. First-principles calculations along the lines of Ref. [5] are needed to specify the strengths and electronic charge distribution of these interaction centers. The analytical theory [2,3] should then be applied using these

realistic potentials. The validity of the theory could then be tested by comparing its results with analyses of the orientational density distribution in the ordered [6,7] and disordered [8] phases.

K. H. Michel
Department of Physics
Universitaire Instelling Antwerpen
B-2610 Wilrijk, Belgium

J. R. D. Copley and D. A. Neumann
Materials Science and Engineering Laboratory
National Institute of Standards and Technology
Gaithersburg, Maryland 20899

Received 23 October 1992

PACS numbers: 61.50.-f, 64.60.Cn, 81.30.Hd

- [1] E. Burgos, E. Halac, and H. Bonadeo, preceding Comment, *Phys. Rev. Lett.* **69**, 3589 (1992).
- [2] K. H. Michel, J. R. D. Copley, and D. A. Neumann, *Phys. Rev. Lett.* **68**, 2929 (1992).
- [3] K. H. Michel, *J. Chem. Phys.* **97**, 5155 (1992).
- [4] M. Sprik, A. Cheng, and M. L. Klein, *J. Chem. Phys.* **96**, 2027 (1992).
- [5] B. Feuston, W. Andreoni, M. Parrinello, and E. Clementi, *Phys. Rev. B* **44**, 4056 (1991).
- [6] W. I. F. David, R. M. Ibberson, J. C. Matthewman, K. Prassides, T. J. S. Dennis, J. P. Hare, H. W. Kroto, R. Taylor, and D. R. M. Walton, *Nature (London)* **353**, 147 (1991).
- [7] A. B. Harris and R. Sachidanandam, *Phys. Rev. B* **46**, 4944 (1992).
- [8] P. C. Chow, X. Jiang, G. Reiter, P. Wochner, S. C. Moss, J. D. Axe, J. C. Hanson, R. K. McMullan, R. L. Meng, and C. W. Chu, *Phys. Rev. Lett.* **69**, 2943 (1992); erratum (to be published).