
ERRATA

**Near Edge X-Ray-Absorption Fine-Structure Determination of Alkyl-Chain Orientation:
Breakdown of the "Building-Block" Scheme
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In the Letter we reported NEXAFS (near edge x-ray-absorption fine-structure) measurements for different thin films containing long alkyl chains, the analysis of which indicated that the so-called "building-block" scheme commonly used to interpret NEXAFS data for larger molecules fails to describe the angular dependence of the C-C resonance at 293.4 eV. We also presented results of *ab initio* SCF-RHF calculations which supported our experimental conclusions. In the meanwhile, however, we discovered an error in the plotting procedure for the transition dipole moments (TDM) as obtained from the *ab initio* calculations. When correctly evaluated the calculations indicate the presence of two resonances with significant TDM's at the energy where experimentally the C-C resonance is observed. This behavior is not predicted by the building-block scheme and has not been observed experimentally, as the C-C resonance half-width (≈ 2.8 eV) is larger than the splitting (≈ 0.7 eV). From their magnitude and orientation (parallel and perpendicular to the chain axis, respectively, with both of them are in the C-C-C plane) an intensity ratio of 2.2:1 for the C-C resonance at normal incidence versus grazing incidence is obtained, which does not differ significantly from the ratio predicted by the building-block scheme (2:1).

The experimental analysis reported in our Letter, however, is not affected by this error, and the conclusion, namely, that there is a breakdown of the building-block scheme, is still considered correct. Note that a recent report [1] on high-resolution NEXAFS measurements on thin layers of hexatriacontane [$\text{CH}_3(\text{CH}_2)_{34}\text{CH}_3$] on Cu substrates presents virtually the same experimental angular dependence of the C-C resonance.

The discrepancy between the (correctly plotted) SCF-RHF calculations and our experimental data for the orientation of the C-C resonance transition dipole moments is partially related to general problems with the theoretical description of virtual orbitals with energies considerably above (> 3 eV) the absorption-step edge. We would also like to mention that the calculated TDM's show an interesting strong dependency on the site of the core hole. With regard to a better understanding of the theoretical aspects this observation should be further pursued.

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[1] T. Ohta, K. Seki, T. Yokoyama, I. Morisada, and K. Edamatsu, Phys. Scr. **41**, 150 (1990).

**Demixing Phase Transition in a Mixture of Hard-Sphere Dipoles and Neutral Hard Spheres
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It was pointed out to us by Smit and de Leeuw that they have found a similar demixing phase transition in a molecular-dynamics simulation of a mixture of neutral Lennard-Jones particles and Stockmeyer particles [1]. They derive the free energy of mixing from the simulation and find coexisting phases. Also in their system the miscibility gap opens for low dipole concentrations where the dipoles can optimize their arrangements.

[1] S. W. de Leeuw, C. P. Williams, and B. Smit, Mol. Phys. **65**, 1269 (1988); S. W. de Leeuw, B. Smit, and C. P. Williams, J. Chem. Phys. **93**, 2704 (1990).