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# Comment on "Jahn-Teller effect for the negatively charged $C_{60}$ molecule: Analogy with the silicon vacancy"

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We point out that the effective $U$ due to vibrational couplings is a factor of 2 larger than calculated by Lannoo *et al.*, due to off-diagonal interactions neglected in their work.

Lannoo *et al.*[1] found an effective interaction between valence electrons on $C_{60}$ due to Jahn-Teller distortions of magnitude $U = -0.05$ eV. This is twice the energy shift of a single electron in the harmonic approximation, and thus agrees with the single-electron energy shift $\Delta E = -0.024$ eV reported in Ref. 2. We wish to point out here that these calculations neglect significant off-diagonal matrix elements of the electron-vibration coupling. Although Lannoo *et al.* write down a Hamiltonian with off-diagonal matrix elements, they minimize in a space that has a static valence electron and static deformation. In the harmonic approximation, it is equivalent to the perturbation expression

$$\Delta E_{\text{static}} = -\sum_{\alpha} \frac{< i,0|V|i,\alpha >^2}{\hbar\omega_\alpha}$$

where the notation $|i,\alpha >$ is a state with an electron in orbital $i$ and the vibrational wave function with a quantum of excitation in the $\alpha$ mode. The valence electron is in the $t_{1u}$ multiplet of states, and in Ref. 1 the state $i$ was chosen to minimize the energy. However, the full perturbation expression should have an additional sum over final electron states in the $t_{1u}$ multiplet,

$$\Delta E_{\text{full}} = -\sum_{\alpha,j} \frac{< i,0|V|j,\alpha >^2}{\hbar\omega_\alpha} \quad . \tag{1}$$

We have recalculated these quantities using the electron Hamiltonian of Refs. 3 and 4 and the vibrational Hamiltonian of Ref. 5. We find values $\Delta E_{\text{static}} = -0.023$ eV and $\Delta E_{\text{full}} = -0.049$ eV, i.e., a doubling when the off-diagonal terms are included.

These relative magnitudes are easy to understand if one replaces the finite-symmetry group by the full rotation group. The $t_{1u}$ state behaves like a state of orbital symmetry $l = 1$, and the dominant $H_g$ vibration behaves like an $l = 2$ state in a spherical basis. Then the ratio of perturbations would be given by a Clebsch-Gordan coefficient, $\Delta E_{\text{full}}/\Delta E_{\text{static}} = (1020|10)^{-2} = 2.5$.

The effective $U$ should be calculated using the full perturbation formula in the two-particle state with symmetry $t_{1u} \times t_{1u} = A$. This is the state $|A >= \sum_j |jj^* > /\sqrt{3}$. The resulting $U$ is twice $\Delta E_{\text{full}}$, while the corresponding $U$ in the static state $|ii^* >$ is twice $\Delta E_{\text{static}}$.

Thus we agree with Refs. 1 and 2 for the calculations they reported, but the full vibrational contribution to $U$ should be $-0.1$ eV. This is still too small to overcome the Coulomb repulsion and make an attractive interaction that would explain the superconductivity.

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[3] D. Tomanek and M. Schlueter, Phys. Rev. Lett. **67**, 2331 (1991).

[4] G. Bertsch *et al.*, Phys. Rev. Lett. **67**, 2690 (1991).

[5] D. Weeks and W. Harter, Chem. Phys. Lett. **144**, 366 (1988).