Enhanced Permeability of Fluorinated Carbon Nanocages
for Medicine

Pavel V. Avramov and Boris I. Yakobson
Rice University
6100 Main Street, Houston, TX 77005, USA.

Carbon nanocages (buckyball C_{60}, larger fullerenes and nanotubes) could be convenient shells-carriers for radioactive isotopes and other components for a variety of medical applications (treatment, image-contrast, diagnostics, etc.). However, their utility is principally hindered by the difficulties of incorporation of most of the elemental components: the yield of the desired structures X@C is extremely low. This is due to large activation barriers for penetration inside the cages and is often complicated by the binding of the ions to the π-electrons.

Theoretical analysis indicates that such barriers can be reduced if the π-subsystem of electrons is depleted by the covalently attached fluorine (e.g. in a $C_{60}F_{48}$, as shown in the Fig. 1). We have performed preliminary calculations and evaluation of the potential barrier reduction, which appears to be substantial. For example, calculations show that while the hexagon-center entry of a proton H+ has a barrier near 6 eV, the similar trajectory barrier for the fluorinated cage is three times lower, near 2 eV. In fact, approximately the same barrier reduction is attained for the "holes" near the hexagon centers of about 1.5 A size, equivalent to nearly 25% of the cage "surface area".

This suggests that the yield of the endohedral units X@CF must be much higher than that of non-fluorinated X@C. It opens new ways for the efficient synthesis of useful endohedral components by either ion beam irradiation or high-pressure/temperature processing [see for example (1)], following the stage of fluorination that can be achieved by previously described methods (2). Detailed quantum-chemical computations (3) must lead to a more accurate assessment of the yield and required conditions for a series of interesting compositions like X@CF (X=H, T, H_2, Li, Co etc.)
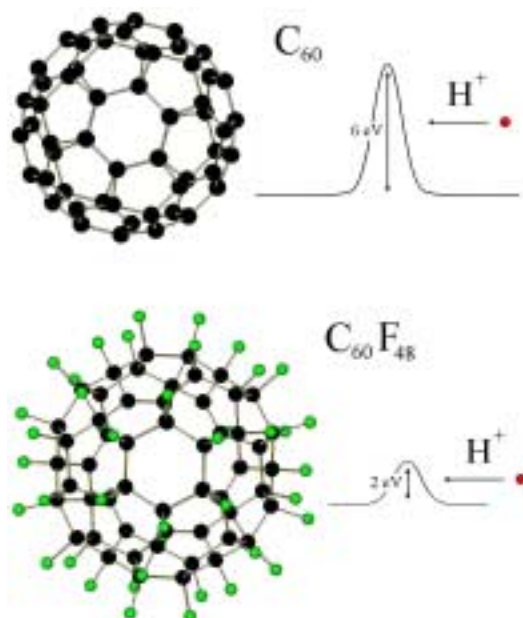
Fig. 1 Illustration of the penetration barrier reduction for a central entry path (proton $\rightarrow$ $C_{60}F_{48}$) obtained by the preceding cage fluorinations.

REFERENCES

1. M. Saunders, R.J. Cross, H.A. Jimenez-Vazquez, R. Shimshi and A. Khong, Science, **271**, 1693 (1996).

2. J. L. Margrave, E. T. Mickelson, R. H. Hauge, and R. E. Smalley, Chem. Phys. Lett., **296**, 188 (1998).

3. P. V. Avramov, G. E. Scuseria, and B. I. Yakobson, work in progress.