On the formation of spherical aromatic endohedral buckminsterfullerene. Evaluation of M@C60(M = Cr, Mo, W) from relativistic DFT calculations

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Endohedral metallofullerenes are key species for expanding the range of viable fullerenes, their versatility, and applications. Here we report our computational evaluation on the formation of spherical aromatic counterparts of the C60 fullerene from relativistic DFT calculations, based on the inclusion of Cr, Mo and W endohedral atoms. The resulting M@C60 endohedral fullerenes are 66-? electron neutral species exhibiting bonding properties and electronic structure mimicking the aromaticity and diamagnetic insulator behavior of alkali-C606- phases. The resulting structures are interesting candidates for further experimental realization as novel neutral building blocks for more flexible nanostructured organic materials, highlighting truly spherical aromatic neutral species retaining the truncated icosahedral structure of the seminal Buckminster fullerene. © the Owner Societies.