Opponent's review of doctoral dissertation
"Endohedral fullerenes: From exotic chemical bonding to molecular electronics"
by Adam Jaroš

The submitted dissertation contains a narrative to a series of four publications (and two in preparation) with a common subject, endohedral fullerenes. The publications are in respected international journals with impact factors and with a significant declared contributions of the candidate. The text of the dissertation is enjoyable to read and I have only a few minor comments or questions.

Page 4, "Compared to graphite, the enthalpy of the formation of C_{60} and C_{70} is 2328 and 2555 kJ/mol higher, respectively. That means that fullerenes possess high kinetic stability." How do you derive 'kinetic' stabilities from enthalpies of formation?

Figure 1.4, wrong ordering in Figure caption.

Page 13, "Since the analytical solution of the Schrödinger equation is, as far as we know, possible only for systems that contain no more than one electron, approximations have to be used." What about hookium? DOI:10.1103/PhysRevA.48.3561

Page 23, integration over volume deserves proper notation in equations 2.39 and 2.41.

Page 23, equation 2.42 is wrong.

Page 26, line 6, gradient is a vector.

Page 29, "Remarkably, the $An_2@C_{80}$ species are the most thermodynamically stable compared to the $An_2@C_{70}$ and $An_2@C_{90}$ species, although it is important to point out that these systems are behind a large kinetic barrier." Can you discuss how to properly compare stabilities of species with different stoichiometries?

Page 38, "Switching voltage that is less than 1.03 V/Å, which should be experimentally achievable." For comparison, what is voltage and distances in an STM experiment?

On overall, I find the submitted dissertation of high quality and I suggest that the candidate is awarded the title of doctor of philosophy.

Filip Uhlík
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