

2A11: EMBEDDED-RING MIGRATION ON GRAPHENE ZIGZAG EDGE.

Russell Whitesides¹, Dominik Domin¹, Romelia Salomón-Ferrer^{1,2},
William A. Lester Jr.^{1,2}, Michael Frenklach¹

¹University of California, Berkeley, USA ²Lawrence Berkeley National Laboratory, USA

Comment by Rubik Asatryan, New Jersey Institute of Technology, USA

asatryan@njit.edu

I think this is an interesting and principal research in the area of soot formation. I would like to focus on the possibility of the formation of charged embedded rings upon doping as I noted during the presentation of this work. Migration of rings can actually be considered as a migration of topological lattice defects via the formation of hypervalent (6-membered) carbon-centered transition states, which can be stabilized by either of electron donors or electron acceptors (e.g., inorganic admixtures well presented in real systems). If the authors would like to include the effect of heteroatoms, my review back to 1988 it might be of interest (it seems to be the latest in this area, not updated by other researchers) on the effect of heteroatoms on the electronic properties of conjugated aromatic systems [1]. Also, I would suggest considering the dimerization mechanism of phenoxy radicals including more general interconversion features [2].

References:

- [1] (a) R.S. Asatryan, N.S. Mailyan, *Polymer Science USSR* (Engl. transl.) 30 (1988) 1135–1141.
(b) R.S. Asatryan, N.S. Mailyan, R.O. Matevosyan, *Theor. & Experim. Chem.* 24 (1989) 457–459.
[2] R. Asatryan, A. Davtyan, L. Khachatryan, B. Dellinger, *J. Phys. Chem. A*, 109 (2005) 11198–11205.

Reply by Russell Whitesides

rawhites@me.berkeley.edu

The focus of our study has been on neutral species, founded on the prevailing view (see [1] and references therein) that ions do not play a dominant role in soot formation in systems of interest. Determining chemical pathways and kinetic parameters for the ion-molecule chemistry is in no way a trivial task [2], and one we do not intend to pursue without more convincing motivation.

References:

- [1] M. Balthasar, F. Mauss, H. Wang, *Combust. Flame* 129 (2002) 204–216.
[2] H. Wang, B. Weiner, M. Frenklach, *J. Phys. Chem.* 97 (1993) 10364–10371.