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**On Desymmetrization and Relativistic Contraction in 4d Atoms.** Boris Udovic, via Timignano 42, 34128 Triest, Italy, boris.udovic@email.si

Perceptible evidences of chemical bond shortening and pyramidalization tendency were observed in particular ensembles around heavy atoms from *3d* to *6d* series of transition elements, which are useful catalysts in Fischer-Tropsch-type synthesis and diamond growth. Among these topics, bond strengthening and desymmetrization phenomena on carbon atoms were detected to some extent also in zwitterionic dimolybdenum(II,II) 3,5-diaminobenzoate tetracarboxylate  $\text{Mo}_2(\text{O}_2\text{CC}_6\text{H}_3(\text{NH}_3^+)_2)_4\text{Cl}_8 \cdot 16\text{H}_2\text{O}$ . Whereas the relativistic contraction of outer *s* orbital produces bond shortening and strengthening in the nearest space, these effects vanish when the *5s* occupation of multiply charged  $\text{M}^{n+}$  cations in oxidation and charge states is not involved. In this context the true electron envelope and the overall reaction dynamics of the formal unit  $\text{Mo}_2^{4+}$  persist to be a rather intriguing question. The synergic presence of the more ligating oxygen atom (O3) by the less ionized carboxylate group and the shortest Mo(1)–O(3) bond inside the octahedral  $\text{Mo}_2\text{O}_8$  cage of low-valent metal atoms intensify the *5s* occupation, which becomes more significant. The repulsion between the electrons in *5s* and *4d* orbitals squeezes together the *4d* orbitals, which experience rather enhanced overlapping processes in multiple metal-metal bond formation with a remarkably blue shifted  $\delta \rightarrow \delta^*$  transition. The bond shortening in terms of *5s* radial contraction and lowering due to relativity shares the increased strength of the dipolar field, which desymmetrizes further the orbital energy and forces the overall electron withdrawing effects in the direction of the chain of vicinal atoms.