The Jahn-Teller Effects in Materials Science, Chemical Reactivity, and Engineering: Novel Findings

I. B. Bersuker, The University of Texas at Austin, Austin, TX 78712, USA, bersuker@cm.utexas.edu

In a review talk, after presenting a general picture of the whole trend, we show some representative (illustrative) examples of direct applications of the Jahn-Teller effects (JTEs, all four modifications) to solving materials science and engineering problems. Below we outline several points in this important and rapidly developing trend (previous reviews see in [1, 2]).

1. Local Jahn-Teller effects continue to be most instrumental in the study of polyatomic systems and their applications as materials for new technologies. Among the latest achievements in this field we notice three important topics: (1) unalienable (fundamental) influence of the JTEs on the structure and properties of local centers in specific crystals that serve as qubits in quantum information storage and computing [3]; (2) use of knowledge on JTEs parameters of local centers in crystals to manipulate (change) their whole sublattices, thus engineering crystal structures with desired properties by means of targeted external influence [4]; and (3) use of external perturbations in different forms to manipulate (engineer) the structure and properties of two-dimensional systems by influencing their PJTE parameters [5].

2. Employing the knowledge that the JTEs are the only source of structural instability of polyatomic systems, and hence the instability of the transition states of chemical reactions are induced by the PJTE-coupling with stable excited states, a whole trend in chemical reactivity is developing, opening new avenues to the theory and its applications to engineering novel reactions; several examples demonstrate the first applications of the theory (see, e.g., [6]). In particular, the application of this PJTE theory to excited-state reactivity opens new ways to studies in photochemistry [7].

3. Applications of the JTEs to cooperative properties in solids, directly employed in materials science, began as early as in 1966 and seem to be inexhaustible. The latest achievements are related to ferroelectricity, flexoelectricity, permittivity, multiferroicity, polar nanoregions, and orientational polarization (see the reviews [8, 9]). Among important unsolved problems in this topic is the absence of computer methods of calculation of electronic structure and properties of solids with JTEs that take into account the specific JTE nuclear dynamics [1].

References

1. a) I. B. Bersuker, The Jahn-Teller and Pseudo Jahn-Teller Effect in Materials Science, *J. Phys. Conf. Series*, 833, 012001 (2017); doi :10.1088/1742-6596/833/1/012001 393; b) I. B. Bersuker, The Jahn-Teller and Pseudo Jahn-Teller Effect in Materials Science, in Recent Studies in Materials Science, Ed. Patrick R. Lind, Nova Science Publishers, 2019, pp. 1-95.

2. I. B. Bersuker, Jahn–Teller and Pseudo-Jahn–Teller Effects: From Particular Features to General Tools in Exploring Molecular and Solid State Properties. Chem. Rev. **2021**, 121, 3, 1463-1512; https://dx.doi.org/10.1021/acs.chemrev.0c00718.

3. Thiering, Gergő; Gali, Adam. The $(e_g \otimes e_u) \otimes E_g$ product Jahn–Teller effect in the neutral group-IV vacancy quantum bits in diamond, *npj Computational Materials*, 2019, *5*, 1-6;

4. Gudkov, V.V., Sarychev, M.N., Zherlitsyn, S. I. V. Zhevstovskikh, N. S. Averkiev, D. A. Vinnik, S. A. Gudkova, R. Niewa, M. Dressel, L. N. Alyabyeva, B. P. Gorshunov & I. B. Bersuker, Sub-lattice of Jahn-

Teller centers in hexaferrite crystal. *Sci. Rep.* **2020**, *10*, 7076-7091; https://doi.org/10.1038/s41598-020-63915-7.
5. I. B. Bersuker, Manipulation of Structure and Properties of Two-Dimensional System Employing the Pseudo Jahn-Teller effect, *FlatChem*, 6, 11–27 (2017); DOI: 10.1016/j.flatc.2017.10.001.
6. Natalia Gorinchoy, Iolanta Balan, Victor Polinger, and Isaac Bersuker, Pseudo Jahn-Teller origin of the proton-transfer energy barrier in the hydrogen-bonded [FHF]-system, Chemistry Journal of Moldova, **2021**, 16(1), 115-120; DOI: http://dx.doi.org/10.19261/cjm.2021.834; Natalia Gorinchoy, Iolanta Balan, Mikhail Gorbachev, Ion Arsene, Victor Polinger, Gheorghe Duca, Isaac Bersuker, Pseudo Jahn-Teller Effect in Transition States of Redox Processes, IGI-Global (USA), 2023.
7. Ya Wang, Yang Liu, and Isaac B. Bersuker, Sudden polarization and zwitterions formation as a pseudo Jahn-Teller effect: A new insight in photochemistry of alkenes, *Phys. Chem. Chem. Phys*., 21, 10677 – 10692 (2019), DOI: 10.1039/C9CP01023H.
8. I. B. Bersuker, The Vibronic (Pseudo Jahn-Teller) Theory of Ferroelectricity. Novel Aspects and Applications, *Ferroelectrics*, 536, 1-59 (2018); https://doi.org/10.1080/00150193.2018.1528919.
9. Isaac B. Bersuker and Victor Polinger, Perovskite Crystals: Unique Pseudo-Jahn–Teller Origin of Ferroelectricity, Multiferroicity, Permittivity, Flexoelectricity, and Polar Nanoregions, *Condens. Matter* **2020**, *5*(4), 68; https://doi.org/10.3390/condmat5040068.

.