THEORETICAL PHYSICS APPROACHES FOR UNDERSTANDING OF MATERIALS: LESSONS FROM Yu. Kh. VEKILOV

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Electronic structure theory is now recognized as highly useful tool for prediction of materials properties, for their understanding, as well as for determination of parameters employed in higher-level modeling. In this talk, novel methodological solutions and exciting applications, which have been inspired by my interactions with Yuri Vekilov will be presented. In particular, development of theoretical tools for simulations of chemical disorder and studies of matter at extreme conditions will be discussed.