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Vibrational, magnetic and many-electron effects in quantitative theory for accelerated materials design IGOR A. ABRIKOSOV, Linkoping University, Sweden, ALENA V. PONOMAREVA, NUST MISIS, Moscow, Russia, ANTON YU. NIKONOV, ANDREY I. DMITRIEV, SVETLANA A. BARANNIKOVA, Tomsk State University and Institute of Strength Physics and Materials Science, Tomsk, Russia, MARCUS EKHOLM, BJORN ALLING, PETER STENETEG, OLLE HELLMAN, Linkoping University, Sweden — We discuss a need to develop modern theory for accelerated materials design, significantly reducing number of approximations in calculations and explicitly taking into account conditions at which materials operate when used in technological applications. We illustrate the need to explicitly account for vibrational, magnetic and many-electron effects by considering several examples, including calculations of phase diagrams for Zr-based alloys, simulations of order-disorder phase transition in Fe-Ni permalloy [1], and estimations of decomposition trends and elastic properties of transition metal nitrides [2-4]. We demonstrate that in this way the accuracy of theoretical predictions can be made comparable to or exceeding the experimental accuracy, significantly increasing usefulness of the theory for the materials design.

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Igor Abrikosov
Linkoping University, Sweden

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