Showcase Applications of DFT in Materials Science

Nikola Koutná

Modelling quantum-mechanical systems with many interacting particles presents a major challenge of modern scientific computing. Firstly formulated in the sixties [1, 2], the Density Functional Theory (DFT) relies on the fact that ground-state properties of atoms, molecules and solids can be extracted from the total charge density. Nowadays, DFT is the state-of-the-art tool to comprehend the electronic structure of matter. This talk illustrates possible applications of DFT within the context of materials science, especially, within the field of hard transition metal nitride and oxide coatings. Examples include stabilisation effect of point defects in metastable phases [3, 4], temperature-induced elimination of soft phonon modes [5], or optimisation of elastic properties and tensile strength for modern engineering devices via superlattice architecture [6, 7, 8]. When possible, theoretical predictions are discussed within the context of experimental data.

[1] P. Hohenberg and W. Kohn. Inhomogeneous electron gas. *Physical Review*, 136(3B):B864, 1964.

[2] W. Kohn and L. J. Sham. Self-consistent equations including exchange and correlation effects. *Physical Review*, 140(4A):A1133, 1965.

[3] Nikola Koutná, David Holec, Ondřej Svoboda, Fedor F Klimashin, and Paul H Mayrhofer. Point defects stabilise cubic Mo-N and Ta-N. *Journal of Physics D: Applied Physics*, 49(37):375303, 2016.

[4] C. Koller, N. Koutná, J. Ramm, S. Kolozsvári, J. Paulitsch, D. Holec, and P. H. Mayrhofer. First principles studies on the impact of point defects on the phase stability of $(Al_xCr_{1-x})_2O_3$ solid solutions. *AIP Advances*, 6(2):025002, 2016.

[5] N. Koutná, P. Erdely, S. Zöhrer, R. Franz, Y. Du, S. Liu, P. H. Mayrhofer, and D. Holec. Experimental chemistry and structural stability of $AlNb_3$ enabled by antisite defects formation. *Materials*, 12(7):1104, 2019.

[6] N. Koutná, P. Řehák, Z. Chen, M. Bartosik, M. Fallmann, M. Černý, Z. Zhang, M. Friák, M. Šob, P. H. Mayrhofer, and D. Holec. Correlating structural and mechanical properties of AlN/TiN superlattice films. *Scripta Materialia*, 165:159–163, 2019.

[7] J. Buchinger, N. Koutná, Z. Chen, Z. Zhang, P. H. Mayrhofer, D. Holec, and M. Bartosik. Toughness enhancement in TiN/WN superlattice thin films. *Acta Materialia*, 172:18–29, 2019.

[8] N. Koutná, R. Hahn, J. Zálešák, M. Friák, M. Bartosik, J. Keckes, M. Šob, P. H. Mayrhofer, and D. Holec. Point-defect engineering of MoN/TaN superlattice films: A first-principles and experimental study. *Materials & Design, in press*, 2019.