Name: Jon Andreas Støvneng
Born: October 15, 1962
Nationality: Norwegian
Present position: Associate professor
Academic degree: Dr.ing.

Work experience: Postdoc at NORDITA, Copenhagen (January 1991 - December 1992); NFR postdoc at Department of physics, NTH, Trondheim (January 1993 - December 1994); Researcher at Department of chemical engineering, NTH/NTNU and Statoil Research Centre (Januray 1995 - December 2002); Associate professor (temporary position) at Department of physics, NTNU, Trondheim (January 2003 - December 2004); Associate professor at Department of physics, NTNU, Trondheim (since January 2005); Deputy Head at Department of physics, NTNU, Trondheim (since September 2009); Leader of Educational Committee at Department of physics, NTNU, Trondheim (since 2005)

Fields of interest and present research activities: Computational physics and chemistry, primarily density functional theory (DFT) applied to problems within catalysis and condensed matter physics. Focus preferably on systems of experimental interest in the physics and chemistry departments at NTNU. Recent and present research activities:

1. Adsorption of atoms and small molecules on surfaces of α-Cr_2O_3. Chromium oxide has a variety of applications, ranging from catalyst in petrochemistry to corrosion protection on stainless steel. Of particular importance, therefore, is a thorough understanding of the interaction of chromium oxide surfaces with different atoms and molecules. (People: Ø. Borck, K. N. Nigussa, K. L. Nielsen)

2. Parametrization of a reactive forcefield (ReaxFF) for III-V and group IV semiconductor materials. When the target is the dynamics of large, reactive systems, quantum mechanical methods like DFT are computationally too expensive. An alternative, then, is to construct an empirical forcefield which allows the breaking and formation of chemical bonds - a socalled reactive forcefield. Accurate DFT calculations are initially performed on small molecules and perfect crystals, and the DFT results are used as input for parametrization of the forcefield. (People: O. Frisk, M. I. Søby, P.-O. Åstrand, A. v. Duin, K. A. Jensen)

3. Parametrization of a reactive forcefield (ReaxFF) for ferroelectric perovskites. See 2. above. In this project, the materials that are studied contain Pb, Sr, Ti and O. Of particular interest is the structure of the $SrTiO_3/PbTiO_3$ interface. (People: G. Oftedal, K. T. Olsen, A. v. Duin, Ø. Borck)

4. Structure and reactivity of Ce-Pt surface alloys. Experimental reports on adsorption of CO on Ce-Pt surface alloys are addressed with DFT calculations, which suggests that the amount of Ce coverage affects the type of surface alloy structure, and hence the reactivity to CO. (People: K. N. Nigussa)

5. Interaction of oxygen with pure and K-doped NiTi shape memory surface alloys. Substitution of Ni by K near the surface is found to enhance the formation of TiO_2 at the expense of TiO, and increase the stability and facilitate the growth of thicker oxides on the NiTi surfaces. This is of importance for the biofunctionality of the alloy. (People: K. N. Nigussa)

6. Hydrogen transfer and hydroxy rotation reactions in vitamin E. On the basis of DFT calculations, it is concluded that electron donation from the heterocyclic ring is an essential ingredient to account for the antioxidant property of vitamin E. (People: R. Aurlien, T. B. Melø)

7. Copper nanoparticles, for applications within catalysis. (People: T. Kristiansen, K. Mathisen, M. A. Einarsrud, D. Nicholson)

8. Chromium oxide and chromium carbide surfaces, for absorption of methane. (People: K. M. Skjelbred, S. Andersson, P.-O. Åstrand, T. van Erp)

Membership in academic and professional committees, scientific review work including peer-review, and other professional merits: Referee in Physical Review Letters, Physical Review A/B/E, and Organometallics. Referee for the Austrian Science Fund (2009). Pedagogical prize from The Faculty of Natural Sciences and Technology, NTNU in 2007. Current leader of the project "iPython Notebook in Physics Education" (P75/2015), supported by Norgesuniversitetet (project period 2015 - 2016).

Doctoral students presently under supervision: Kristin M. Skjelbred, Department of chemistry (co-supervisor)

Selected academic and professional publications 2005 - 2015:

- Eilertsen, J. L.; Støvneng, J. A.; Ystenes, M.; Rytter, E.; Activation of Metallocenes for Olefin Polymerization As Monitored by IR Spectroscopy. Inorganic Chemistry **44**, 4843 (2005)

- Eide, O.-K.; Ystenes, M.; Støvneng, J. A.; Eilertsen, J.L.; Investigation of ion pair formation in the triphenylmethyl chloride-trimethyl aluminium system, as a model for the activation of olefin polymerization catalyst. Vibrational Spectroscopy **43**, 210 (2007)

- Möller, A. C.; Blom, R.; Swang, O.; Hannisdal, A.; Rytter, E.; Støvneng, J. A.; Piel, T.; On the nonsingle-site character of bis(2-dimethylsilyl-indenyl)zirconium(IV) dichloride/MAO and bis(2-trimethylsilyl-indenyl)zirconium(IV) dichloride/MAO: Polymerization characteristics and mechanistic implications. Journal of Physical Chemistry A **112**, 4074 (2008)

- Nigussa, K. N.; Støvneng, J. A.; Oxidation of pure and potassium-doped NiTi shape memory surface: A density functional theory investigation. Phys Rev B **82**, 245401 (2010)

- Nigussa, K. N.; Støvneng, J. A.; Theoretical investigation of the interaction of oxygen with pure and K-doped NiTi shape memory surface alloys. Computer Physics Communications **182**, 1979 (2011)

- Nigussa, K. N.; Nielsen, K. L.; Borck, Ø.; Støvneng, J. A.; Adsorption of hydrogen, chlorine, and sulfur atoms on α-Cr_2O_3(0001) surfaces: A density functional theory investigation. Corrosion Science (2011), doi:10.1016/j.corsci.2011.07.005

- Kristiansen, T.; Støvneng, J. A.; Einarsrud, M. A.; Nicholson, D. G.; Mathisen; K.; There and Back Again: The Unique Nature of Copper in Ambient Pressure Dried-Silica Aerogels. J. Phys. Chem. C **38**, 116 (2012)

- Skjelbred, K. M.; Åstrand, P.-O.; Støvneng, J. A.; and Andersson, S.; Surface and bulk properties of chromium oxide: Implications for reduction by methane. AIP Conf. Proc. **1702**, 090061 (2015); doi:10.1063/1.4938869

- Hiis Hauge, E.; Støvneng, J. A.; Grunnleggende fysikk - klassisk mekanikk og varmelære. Tapir akademisk forlag (2010). (Book)