CeNT CENTRE OF NEW TECHNOLOGIES

UNIVERSITY OF WARSAW

invites to a seminar by

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In-silico design and mechanistic studies of metathesis catalysts

12th October 2017 at 12 p.m.

Venue: Centre of New Technologies, Banacha 2C,
Lecture Hall 0142 (Ground floor)

Host: Prof. Joanna Kargul

Metathesis reaction itself has been named as "emerging green technology" by the Royal Academy of Science during the 2005 Nobel Prize award and was quickly adopted by research groups as a basic strategy for the synthesis of C-C bonds. The ability of this method for the selective substitution of atoms between two molecules allows for generation of chemical systems with the desired properties. This is particularly important for complex compounds such as natural compounds , as well as new heterocyclic and macrocyclic compounds.

The overwhelming number of applications of metathesis reaction nowadays is truly remarkable, especially considering the short time since it was first observed. A large number of olefin metathesis applications in various industries have been growing over the years. The synthesis of numerous complex organic molecules and materials, such as pharmaceuticals, polymers, agrochemicals and natural products, has been facilitated by well-defined catalysts. Despite the wealth of accumulated research, there has been an ever increasing academic interest in this area over the years.

Our group is using computational chemistry tools to rationally design new metathesis catalyst, answer some elusive questions regarding the mechanism, and improve catalysts through systematic *in-silico* tuning of their properties. In this talk we will present the methodology we use, as well as a number of case studies which lead to the design of new catalyst and/or a better understanding of their mechanisms of action.

*Trzaskowski et al. Organometallics **2013**, 32, 3625; Pazio et al. Organometallics **2015**, 34, 563; Pazio et al. Dalton Trans. **2015**, 44, 20021; Trzaskowski et al. RSC Adv. **2016**, 6, 21423; Trzaskowski et al. Catal. Commun. **2016**, 86, 133; Gawin et al. ACS Catal. **2017**, 7, 5443; Grudzień et al. Dalton Trans. **2017**, 46, 11790.*

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