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Whole New Landscapes (Award Lecture, SCS Honorary Member 2016)

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This story is about changes and connections in chemistry research. The new places, the new people, the new discoveries lead you into an ever-evolving yet connected world. Curiosity, passion, luck and perseverance propel you forward. Perspectives are constantly changing, but by looking back the pattern emerges.

This presentation will explore the author and his groups' research in organometallic chemistry and catalysis – from metal vapor synthesis to asymmetric catalytic C-H activation.[1]

[1] See: https://www.unige.ch/sciences/chiorg/kundig/publications.

Development of commercial organic additives for the grinding of inorganic solids

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Grinding aids have been used successfully for decades in the production of many materials, such as cements, ceramics, pigments etc. These products reduce the energy needed for grinding, which in the case of cement has major environmental implications worldwide. This is primarily due to the tremendous amounts of cement produced and also 30% of the associated electricity energy consumption is used for grinding. For example, yearly global savings of electrical energy achieved thanks to grinding aids are on the order of the energy generated by 2-3 nuclear power plants. However, even more importantly, these compounds make it possible to change cement compositions to produce materials of equivalent performance with much lower environmental impact. To give a scale of the environmental impact of cement production and the gains that can be made by reducing it, we point out that about 30-40% of the CO_2 reductions targeted by Switzerland in the Kyoto protocol have been achieved by the cement industry alone.

In this lecture, we examine the question of how to optimize these grinding aids linking molecular insight into their working mechanism. For this, we start by recognizing that surface and interfacial properties play an important role during the comminution process of inorganic minerals.[1-5] We focus on the clinker phases of ordinary Portland cement onto which grinding aids can adsorb during clinker grinding. For this, we apply molecular dynamics simulations using validated molecular models to study the interactions of various types of chemical additives with clinker minerals. A key role is hereby played by the quantitative representation of ionic versus covalent contributions to bonding in cement minerals via atomic charges. We establish the validity of molecular models and associated force field parameterization by precise atomistic simulation of structural, dynamic, surface, mechanical and thermal properties of minerals in agreement with available X-ray data, IR spectra, cleavage energies, and measured elastic constants.[6] This has led us to an understanding breakthrough of the molecular interactions of grinding aids on inorganic mineral surfaces at an atomistic level. Very importantly our molecular modeling results properly rank the performance of grinding aids as reported from full-scale cement production. Computed agglomeration energies of cement particles with various adsorbed organic compounds correlate with the reduction in surface forces in the form of experimental data on grinding efficiencies. Such knowledge paves the way to molecular design of chemical additives of improved performance. Finally, we will discuss the implications for industrial development of having research changing the conceptual thinking on how specific products function. We will finish by expanding these thoughts to the question of how to put a value on an “invaluable contribution”.

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