Applicant: Cleuren Bart, Hasselt University (Belgium)
Visit to: Ralf Eichhorn, Nordita, Stockholm (Sweden)

Scientific Report

As stated in our project proposal, the focus of our collaboration is on the efficiency of energy conversion at a small scale. We considered (i) the conversion of kinetic energy into translation/rotational motion of a granular motor and (ii) chemical energy conversion by pumping ions against their chemical energy gradient by means of an ion channel. The aims of the visit were, for the system (i) to determine (analytically and by simulations) the efficiency in the Brownian limit as a first step towards its optimization, and for system (ii), to set up the model and derive first results for the efficiency.

For the granular motor model, we successfully calculated the efficiency in the Brownian limit (heavy motor mass), and this both for the translational and rotational motors. The rotational variant is of particular interest in view of future experimental verification. As was expected, the efficiency is rather low in the Brownian limit. However, the analytical formula allows for an optimization of the motor shape in order to increase the efficiency. This optimization procedure is the subject of future work. In order to verify our calculations, and to test their robustness against non-ideal modifications, molecular dynamics simulations were performed. In these simulations, the exact microscopic dynamics is considered, allowing for example to investigate the influence of recollisions between motor and gas particles. The first preliminary results are in agreement with our calculations. In order to obtain a profound understanding of the efficiency of granular motors, we plan to undertake further extensive computer simulations allowing us to investigate parameter regimes that can not be accessed by our theoretical calculations. These regimes include a small restitution coefficient (strongly dissipative collisions, introducing a significant increase in recollisions), heterogeneous motors for which the restitution coefficient varies along the surface of the motor, and the non Brownian limit. Our main results obtained during the visit will be further extended by the results of the computer simulations, and we expect this to result in a publication.

For the conversion of chemical energy by means of an ion channel, we set up a model with two ion species and two internal positions inside the ion channel. This is a minimal model in so far as it allows the two species to be simultaneously be present inside the channel. The master equation describing the dynamical features of this model was derived, and the first results of the ion currents were obtained. In view of the large amount of parameters yet undetermined, a careful selection is needed in order not to lose the basic features of the model, and to reduce the computational effort. The following steps include the calculation of the efficiency and its analysis in terms of the Onsager coefficients and the so-called degree of coupling between the two ion currents. A further aspect will be the selectivity of the ion transport through the channel with respect to different ion species.

In order to proceed with these projects, we have informally agreed upon a visit of Ralf Eichhorn to Hasselt University early next year.