Overview of the PhD student activities in the Chemistry program in the field of Environmental Chemistry: 2014/15

Student (given name and surname)	Joseph K´Ekuboni MALONGWE
Supervisor (given name and surname)	Professor Petr Klán
Consultant (given name and surname)	
Beginning of the study (month/year)	December 6th, 2011
Form of study (delete where appropriate)	Present (internal)

Summary of yearly research results (15 lines maximum)

1. An experimental – computational method was used to investigate the spectroscopic behavior of naphthalene on the surface of ice grains. UV-vis diffuse reflectance and fluorescence spectroscopies of naphthalene combined with DFT and ADC(2) calculations provided evidence for the occurrence of excited-state associates. The measured and calculated bathochromic shifts of the S0→ S1 electronic transitions related to naphthalene dimers or naphthalene–ice interactions did not exceed 3 nm. The bands observed in the emission spectrum of frozen naphthalene solutions were assigned to excited dimers of different mutual orientations. Frozen solutions of naphthalene was exploited to demonstrate both the absence of considerable bathochromic shift and a strong tendency to aggregate.
2. Experimental studies of the heterogeneous ozonation of pyrene at the air-ice interface on artificial snow prepared by shock-freezing technique had shown that this reaction follows Langmuir – Hinshelwood type mechanism. Pyrene molecules were largely ejected to the surface of snow grains and available to react with the gas – phase reagent ozone. The lower k_{O3} value for pyrene at 258 K suggested decreased partitioning of ozone at 258 K than 188 K.

Internship abroad (place, start date, duration)

Publication activities

Number of peer-reviewed articles in impacted journals	2
Number of conference (oral/poster) presentations	
Number of other publishing activities (books, book chapters, patents etc.)	
Public lecture in English (delete where appropriate)	yes

The most important results (5 maximum, show the impact factor of the journal):

1	Apparent Rate Acceleration of the Heterogeneous Reaction of Ozone with Alkene at the Air – Ice Interface at Lower Temperature, **in Environ Sci Technol, 2013 Jul2; 47 (13): 6773-80**. **Impact Factor : 5,257**
2	Spectroscopic Properties of Benzene at the Air–Ice Interface: A Combined Experimental–Computational Approach, **in The Journal of Physical Chemistry, A 2014, 118, 7535−7547** **Impact Factor: 4,814**
3	Spectroscopic Properties of Naphthalene on the Surface of Ice Grains Revisited: A Combined Experimental–Computational Approach, **submitted in The Journal of Physical Chemistry** **Impact Factor: 4,835**
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