Grenoble, April 23rd 2012

Dear Mark,

This is to recommend Dr. Jerome Roy for the post of a programming researcher available at the ILL. I work as a second scientist at the ID32 beamline at the ESRF and it was always a pleasure to work with and co-supervise Jerome for more than 4 years. He was first a post-doc and then a young scientist in our group. He was the person who introduced me into the operation of our beamline as he's been there since 1 year before I arrived.

Since the beginning Jerome showed a particular interest in and understanding of the technical and computing issues of the beamline operation. This more technical focus has distracted him sometimes from more scientific work. During his stay at ID32 he has developed from a rather impatient and unfocused post-doc into a persistent and concentrated young scientist who keeps track of the scientific goal even when deeply immersed in the technicalities of the subject. During his last appointment as an executive leader of a long-term project (X-ray standing wave on zeolite microcrystals) he has shown capabilities to manage a technically very challenging scientific project – by organizing instrument development and/or loans, by careful planning and developing various experimental approaches, and especially by optimizing those by computer simulations. Despite meagre scientific results from his mission he was able to produce important results in the form of technique-based papers.

One of the main activities of Jerome during his young scientist appointment was development of Python-based data analysis and simulation code for X-ray standing wave technique called PyXSW. The X-ray standing wave (XSW) is a technique that combines structural and spectroscopic information about matter thus allowing to refine crystal structures and adsorbate geometries with chemical state and atomic species selectivity. The data analysis requires determination of the phase of the standing wave which is not possible by simple fitting to an analytical function but it accessible only via dynamical theory of diffraction and includes the simulation of the phase change over the whole optical path. Development of a computer code for data analysis thus requires extensive knowledge in optics and in scientific computing. Based on the zeolite project and other users' demands, Jerome has developed, almost on his own, a very versatile package in Python that illustrates his abilities in scientific programming. Being a Python-literate scientist (and a contributor to one of the tool scripts in PyXSW) I also appreciate his approach that uses the maximum of available resources without duplicating them (DABAX database, CIF structure files, standard ESRF data formats, least-square fitting routines) which is a "good practice" in scientific computing sometimes neglected by scientists. Jerome's code is very well documented including a tutorial and examples which allow even a beginner Python user to write personalized scripts that go beyond capabilities of other existing XSW data analysis codes. I will not exaggerate if I say that with this package one can analyze any XSW data today. For me, it has become an indispensable tool in my scientific work.

Jerome has a very strong sense of collaboration and appreciates mutual help and distribution of tasks between scientists in a project. He can work both independently or in collaboration, depending on the requirements of the problem. He usually tries to find a solution alone (or, in

the case of Python, by documentation and forum search) but he is not afraid to ask others for help on more complex issues. As an example I can mention his collaboration with J. Kieffer and C. Ferrero (Scientific Computing Group at the ESRF) for issues including the code's internal structure, maintenance and distribution.

I think Jerome is a very suitable candidate for the proposed job. He will be very attentive to the main issue of the project which is, in my view, the various types of data (and possible resulting data formats) to deal with. Having experience from a technique that combines two (or more) very different signals (diffraction and various spectroscopic signals) he will be able to generalize and anticipate needs of the software to develop. He also has got experience from developing scientific software for a user community, not only for himself.

I highly recommend Jerome for the announced post not only based on his scientific computing capabilities but also taking into account his collaboration skills.

Should you need more information, don't hesitate to contact me by phone at 04.76.88.27.76 (office) or 04.76.88.26.65 (beamline), I will be happy to discuss my recommendations in more detail.

Sincerely,

Blanka Detlefs

scientist at ID32 beamline, ESRF