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講演題目	**Structure modeling of quasicrystals from a real-space perspective**
講師	**Dr. Radoslaw Strzalka** （Research fellow, Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Krakow, Poland）
日時	平成２９年６月１５日（木） １５：００～１６：００
場所	工学部 Ａ１－１７室

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Structure modeling of quasicrystals from a real-space perspective

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In my seminar presentation I will discuss the statistical method of structural analysis of quasicrystals and other aperiodic systems [1,2], and show the results obtained by our group from AGH Krakow in recent years. I will start with short introduction of myself and my collaboration with Prof. H. Takakura [3]. After the introduction to the statistical method (concept of the average unit cell, AUC) and general overview, the focus will be put on two points: (*i*) derivation of the structure factor for icosahedral quasicrystals (iQCs) based on the Ammann tiling, and (*ii*) including atomic disorder in the statistical modeling of quasicrystals. The structure factor for Ammann tiling with arbitrary decoration is ready to use in a refinement program [4]. The subdivision of the AUC into 10 independent regions has been done and the structure factor has been derived with separation of "lattice" part and "atomic" part. Also a correctness of the structure factor was quantitatively confirmed by application to simple decoration scheme of iQCs [5]. Statistical method in natural way gives insight to phonons and phasons present in the system. Including these phenomena in structure refinement is easy if statistical approach is used, and it is carried out at the structure factor construction stage [6,7]. Subtopics (*i*) and (*ii*) will be discussed in more details.

In the last part of my talk I will discuss results obtained from my collaboration with Dr. M. Mihalkovic (SAS, Bratislava, Slovakia), which deal with perpendicular-space modeling of quasicrystals from a real-space perspective [8]. Three subjects will be plotted: canonical-cell-tiling decomposition of the Katz-Gratias model of iQCs, improving 12-fold packing models by means of complete space filling with exclusion of short atomic distances at the same time (new occupation domain, OD, is needed), and developing surface-connectedness Hamiltonian in Monte Carlo simulation for controlling the shape of new ODs. This project is still ongoing.

All presented results are obtained by members of the Prof. Janusz Wolny group in AGH Krakow, Poland, in collaboration with academic centers in Slovakia, Switzerland and Japan.

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