

Theoretical tasks for understanding skutterudites

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Filled skutterudites show a rich variety of interesting phenomena, which have been investigated intensively in this priority-area project for two years. When one looks into the ever accumulating pile of information, one may feel dazzled and overwhelmed. Thus the theoretical group was formed within the project by the need to have a compass for sailing into the rich but perilous sea of skutterudites and, hopefully, to organize the research project as effective as possible in the remaining two years. The team consists of theoreticians who will work on:

- (A) investigation of electronic structure,
- (B) building microscopic models,
- (C) investigation of superconductivity,
- (D) investigation of transport phenomena,
- (E) investigation of local correlation effects.

More specifically, I would take the following topics as representatives among many aspects of skutterudite systems:

1. Heavy electrons with plural number of f electrons

Pr and Sm skutterudites show heavy masses which may originate from mechanisms other than magnetic Kondo interactions. Especially the role of unharmonic phonons is to be clarified.

2. Superconductivity

The nature of pairing in $\text{PrOs}_4\text{Sb}_{12}$ remains unclear. On the basis of theoretical models, we shall propose experiments to identify the pairing. We hope to suggest possible new superconductivity in other skutterudites, considering the role of the unharmonic phonons.

3. Borderline between localized and itinerant behaviors

$\text{PrFe}_4\text{P}_{12}$ shows a metal-insulator (M-I) transition under pressure. The insulating state is reminiscent of that in $\text{PrRu}_4\text{P}_{12}$, but is easily destroyed by magnetic field. Comparison with the M-I transition in $\text{SmRu}_4\text{P}_{12}$ should be made.

4. Scalar and multipole orders

It now appears that $\text{PrFe}_4\text{P}_{12}$, $\text{PrRu}_4\text{P}_{12}$, and $\text{SmRu}_4\text{P}_{12}$ keep the cubic symmetry even in the ordered phase. This shows that the order parameters are point-group scalars in all three cases. In the Pr cases, this scalar does not break the time-reversal symmetry, hence 4-th and 6-th rank tensors form the scalar. On the other hand, the order in $\text{SmRu}_4\text{P}_{12}$ seem to break the time-reversal. Then the pseudo-scalar with the xyz -symmetry (octupole) is the best candidate. We shall propose experiments which may identify the order parameters.

5. Transport and thermoelectromagnetic properties

Not only the equilibrium properties, but transport properties have their own interest. In addition to the electrical resistivity, investigation should be made on thermomagnetic and thermoelectric properties. It has recently been reported that URu_2Si_2 shows a gigantic Nernst coefficient. Skutterudites with hidden order may also show significant transport anomaly.

It is clear that there are other important and interesting problems than those mentioned above. In addition to our theoretical team, there are a few independent theoretical projects adopted from public proposals. In addition to this meeting, we plan to organize small workshops including all these people to promote the investigation.