

**Franco-Japanese PhD position**  
**Characterising semiconductors for photovoltaics applications using EPR and DFT**

Funding is available for a PhD position starting before November 2020, working under the direction of Dr. Serge Gambarelli at the CAMPE team, CEA Grenoble (University Grenoble Alpes, France) and Prof. Takashi Suemasu at semiconductor science and device team (University of Tsukuba, Japan). The student will be enrolled at University Grenoble Alpes, but the PhD will be validated by both UGA and University of Tsukuba (viva through English). The student will spend approximately 50% of their time in each University.

The research topic relates to barium silicide ( $\text{BaSi}_2$ ), a promising semiconductor for photovoltaic applications. Prof. Suemasu's laboratory (Tsukuba) is the world leader producing thin-film devices with this compound (1, 2). To optimise the efficiency of these devices, it is essential to understand and control the nature and concentration of defects in the thin-film. Dr. Gambarelli's group specialises in advanced electron paramagnetic resonance (EPR) and density functional theory (DFT) calculations (3, 4). A previous collaboration between the two laboratories demonstrated that advanced EPR used in combination with DFT computation was ideally suited to analysing and understanding defects in  $\text{BaSi}_2$ .

Over the course of this PhD, the student will develop and use innovative advanced EPR methods to study and identify defects, both in bulk  $\text{BaSi}_2$  and in thin-film devices to produce systems with improved capabilities. In parallel, another student will be working on a related project, also conducted between Grenoble and Tsukuba.

Candidates should have an interest in semiconductors and physical chemistry. Previous experience in EPR and DFT would be a plus. The salary is approximately €1760/month for a total duration of three years.

1: T. Suemasu and Noritaka Usami. Exploring the potential of semiconducting  $\text{BaSi}_2$  for thin-film solar cell applications. *J. Phys. D: Appl. Phys.* 50 (2017) 023001.

2: Z. Xu et al., Marked enhancement of the photoresponsivity and minority-carrier lifetime of  $\text{BaSi}_2$  passivated with atomic hydrogen. *Physical Review Materials* 3 (2019) 065403.

3: T. Sato et al. Investigation of native defects in  $\text{BaSi}_2$  epitaxial films by electron paramagnetic resonance. *Applied Physics Express*, 12 (2019) 061005.

4: G. Sicoli et al. Fine-tuning of a radical-based reaction by radical S-adenosyl-L-methionine tryptophan lyase. *Science* 351 (2016) 1320.

**Candidates should send:**

A CV (academic transcript, experience, other interests) and cover letter to:

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