

## Synchrotron Radiation Applications Workshop on Computational & Experimental Materials Physics (COMPEX2018)

Computational Materials Physics Project, Synchrotron Light Research Institute (SLRI)

23-24 July 2018 at Thammasart University (TU), Rangsit

| Time          | July 23, 2018                                                                                                                                                                                                                                             |
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| 08:30 – 09:00 | Registration<br>(Department of Engineering, TU)                                                                                                                                                                                                           |
| 09:00 – 09:15 | Welcome ( <b>Assoc. Prof. Dr.Wanchai Phaijitrojana</b> , TU)                                                                                                                                                                                              |
| 09:15 – 10:00 | Comp I: Structure Determinations: When Computations meet Experiments<br>@SLRI ( <b>Dr.Wutthikrai Busayaporn</b> , SLRI)                                                                                                                                   |
| 10.00 – 11.00 | Exp I: Synchrotron X-ray Absorption Spectroscopy as an Advanced<br>Characterization Technique in Materials Physics and Materials Science:<br>an Experimental Approach ( <b>Prof. Dr.Rattikorn Yimnirun</b> , VISTEC)                                      |
| 11:00 – 11:15 | Break I                                                                                                                                                                                                                                                   |
| 11.15 – 12.00 | Comp II: Local Structure Evolution in AlN Thin Film Studied by Soft X-ray<br>Absorption Spectroscopy and 1 <sup>st</sup> Principle Calculation<br>( <b>Dr.Wutthigrai Sailuam</b> , Rajamangala University of Technology ISAN, Khon<br>Kaen Campus, RMUTI) |
| 12.00 – 13.00 | Lunch                                                                                                                                                                                                                                                     |
| 13.00 – 13.45 | Exp II: TBA<br>( <b>Dr.Mati Horprathum</b> , National Electronics and Computer Technology<br>Center, NECTEC)                                                                                                                                              |
| 13.45 – 14.45 | Comp III:<br>( <b>Assoc. Prof. Dr.Wanchai Phaijitrojana</b> , TU)                                                                                                                                                                                         |
| 14.45 – 15.00 | Break II                                                                                                                                                                                                                                                  |
| 15.00 – 15.45 | Exp III: Nanoshelled Silver Supported-TiO <sub>2</sub> Enhancement of Elementary<br>Mercury Adsorption ( <b>Dr. Pongtanawat Khemthong</b> , National<br>Nanotechnology Center, NANOTEC)                                                                   |
| 15:45 – 16:30 | Discussion                                                                                                                                                                                                                                                |

| Time          | July 24, 2018                                                                                                                                                                                                 |
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| 08:30 – 09:00 | Registration (TU) (by SLRI-CMP & RMUTI)                                                                                                                                                                       |
| 09:00 – 10:30 | Theory of Density Functional Theory, DFT<br>- Workshop overview<br>- Density functional theory (DFT)<br>( <b>Dr.Wutthigrai Sailuam</b> , RMUTI)                                                               |
| 10.30 – 10.45 | Break                                                                                                                                                                                                         |
| 10:45 – 12:00 | VASP Basics:<br>-Basic Linux command<br>- Input and output files<br>- Density of states and band structure calculation (DOS)<br>( <b>Dr.Wutthigrai Sailuam</b> , RMUTI & <b>Dr.Maneerat Chotsawat</b> , SLRI) |
| 12.00 – 13:00 | Lunch                                                                                                                                                                                                         |
| 13:00 – 14:00 | Basic theory of X-ray Absorption Spectroscopy, XAS<br>( <b>Dr. Athipong Bootchanont</b> , Rajamangala University of Technology, Thanyaburi, RMUTT)                                                            |
| 14:00 – 14:15 | Break                                                                                                                                                                                                         |
| 14.15 – 16.30 | Introduction to FEFF<br>-Athena / Download and Installation/ Hand on/<br>Example simulations<br>( <b>Dr. Athipong Bootchanont</b> , RMUTT)                                                                    |