

## Program of MMSNF-6

### First day, December 13, 2007

| Time  | Author   | Title  |
|---|--|--|
| 9:00 ~ 9:50                                     | Registration   |  |
| 9:50 ~ 10:00                                    | Shuichi Iwata (Tokyo Univ.)  | Opening  |
| <b>Session I Thermodynamics</b>                 |  |  |
| 10:00 ~ 10:30                                   | <u>I-1</u> J.C. Dumas, C. Martial and C. Guéneau   | Contribution to the thermodynamic modeling of the (U-Pu-C) ternary system in the frame of the FUELBASE Project |
| 10:30 ~ 11:00                                   | <u>I-2</u> C. Guéneau, S. Gossé, S. Chatain, N. Dupin, B. Sundman, J.-C. Dumas, C. Martial, C. Rado, R. Konings, H. Noel | Progress of the FUELBASE project for the development of a thermodynamic database for advanced nuclear fuels    |
| 11:00 ~ 11:30                                   | <u>I-3</u> M. Kurata   | Thermodynamic database for U-Pu-Zr-Np-Am-Fe system, ver.1.0  |
| 11:30 ~ 12:00                                   | <u>I-4</u> M. Hirota, K. Kurosaki, M. Uno, S. Miwa, M. Osaka, K. Tanaka, and S. Yamanaka                                 | Modeling and Calculation of the Phase Equilibria of the Actinides-Oxygen Systems                               |
| 12:00 ~ 13:30                                   | ***** Lunch *****  |  |
| <b>Session II Molecular Dynamics Simulation</b> |  |  |
| 13:30 ~ 14:00                                   | <u>II-1</u> J.Y. Oh, Y.H. Koo, B.H. Lee  | Molecular dynamics simulation of xenon gas behavior in a nuclear fuel  |
| 14:00 ~ 14:30                                   | <u>II-2</u> M. Osaka, J. Adachi, K. Kurosaki, M. Uno, S. Yamanaka  | Molecular Dynamics Study on Defect Structure of Rare Earth-doped Thoria  |
| 14:30 ~ 15:00                                   | <u>II-3</u> K. Kurosaki, M. Katayama, J. Adachi, M. Uno, S. Miwa, M. Osaka, K. Tanaka, and S. Yamanaka                   | Molecular Dynamics Simulation of the Thermal Properties of Minor Actinides-Containing Mixed Oxide Fuels        |
| 15:00 ~ 15:30                                   | ***** Tea Break *****  |  |
| <b>Session III First Principle calculations</b> |  |  |
| 15:30 ~ 16:00                                   | <u>III-1</u> M. Freyss, B. Dorado, J. Durinck  | Ab initio study of the behavior of point defects and volatile elements in nuclear fuels                        |
| 16:00 ~ 16:30                                   | <u>III-2</u> Y. Chen, HY Geng, Y. Kaneta, M. Kinoshita, J. Nakamura  | First principle calculations of lattice defects in UO <sub>2</sub> and CeO <sub>2</sub>                        |
| 16:30 ~ 17:00                                   | <u>III-3</u> S. Minamoto, K. Konashi, M. Kato  | First principle calculation of Thermodynamics properties of PuO <sub>2</sub>                                   |
| 17:00 ~ 17:30                                   | <u>III-4</u> T. Nishi, M. Nakada, A. Itoh, C. Suzuki, M. Hirata, M. Akabori  | XAFS study of americium dioxide  |

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**Second day, December 14, 2007**

| Time   | Author  | Title   |
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| <b>Session IV Fuel behavior and simulation codes</b> |   |   |
| 9:30 ~ 10:00   | <u>IV-1</u> E.C. Corcoran, B.J. Lewis, W.T.Thompson | Computed Phase Equilibria and Material Studies for Burnable Neutron Absorbing Materials for the Advanced CANDU Reactor Design             |
| 10:00 ~ 10:30  | <u>IV-2</u> T. Bartel, M. Lusk, V. Tikare           | Numerical Modelling of Gaseous Fission Product Transport at the Microscale  |
| 10:30 ~ 11:00  | <u>IV-3</u> V. Tikare, A. Garcia and T. Bartel      | Numerical Simulation of Diffusive Processes in Thermal Gradients  |
| 11:00 ~ 11:30  | <u>IV-4</u> A. Courcelle                            | Model of Defect Chemistry in (U,Pu)O <sub>2</sub>   |
| 11:30 ~ 12:00  | <u>IV-5</u> P. Cristea, M. Stan                     | Simulations of Coupled Heat and Oxygen Diffusion in Porous Urania Fuel  |
| 12:00 ~ 13:00  | ***** Lunch *****                                   |   |
| 13:00 ~ 13:30  | <u>IV-6</u> M.J. Welland, W.T. Thompson, B.J. Lewis | Simulation of High Temperature Phase Transitions in UO <sub>2+x</sub>   |
| 13:30 ~ 14:00  | <u>IV-7</u> M.S. Veshschunov                        | Application of the MFPR code to analysis of the Japanese tests on irradiated UO <sub>2</sub> fuel microstructure and fission gas release. |
| 14:00 ~ 14:10  | Motoyasu Kinoshita                                  | Closing Remarks   |
|  | *** vacant available time range ***                 |   |
| ~ 15:00  | Koshiba-hall is available till 1500                 |   |