পারমানবিক বিদ্যুৎ কেন্দ্রের চুল্লিতে ব্যবহৃত রক্ষন আবরণের কাঠামোগত বৈশিষ্ট সংক্রান্ত গণনামূলক গবেষণার জন্য কম্পিউটার ক্রয়

ড. মোহাম্মাদ আবদুর রশিদ

সহকারী অধ্যাপক

পদার্থবিজ্ঞান বিভাগ

যশোর বিজ্ঞান ও প্রযুক্তি বিশ্ববিদ্যালয়

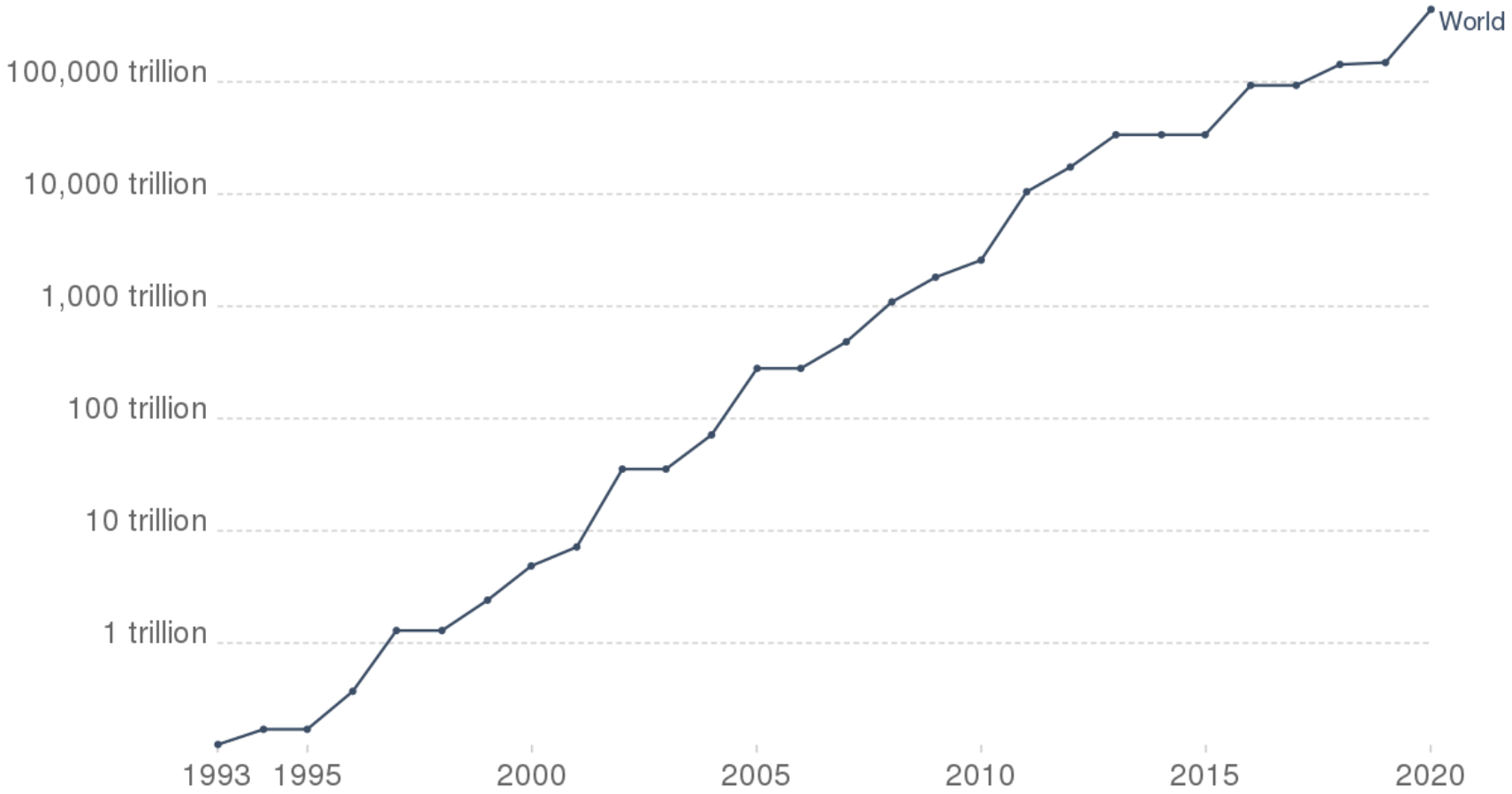
Uses of Computers

- Education & Research
- Communication
- Business
- Healthcare
- Retail and Trade
- Government
- Marketing
- Science
- Publishing
- Arts and Entertainment
- Banking and Finance
- Transport
- Navigation
- Working From Home
- Military
- Social
- Booking Vacations
- Security and Surveillance
- Weather Forecasting
- Robotics

Supercomputer Power (FLOPS), 1993 to 2020

Our World in Data

The growth of supercomputer power, measured as the number of floating-point operations carried out per second (FLOPS) by the largest supercomputer in any given year. FLOPS are a measure of calculations per second for floating-point operations. Floating-point operations are needed for very large or very small real numbers, or computations that require a large dynamic range. It is therefore a more accurate measured than simply instructions per second.



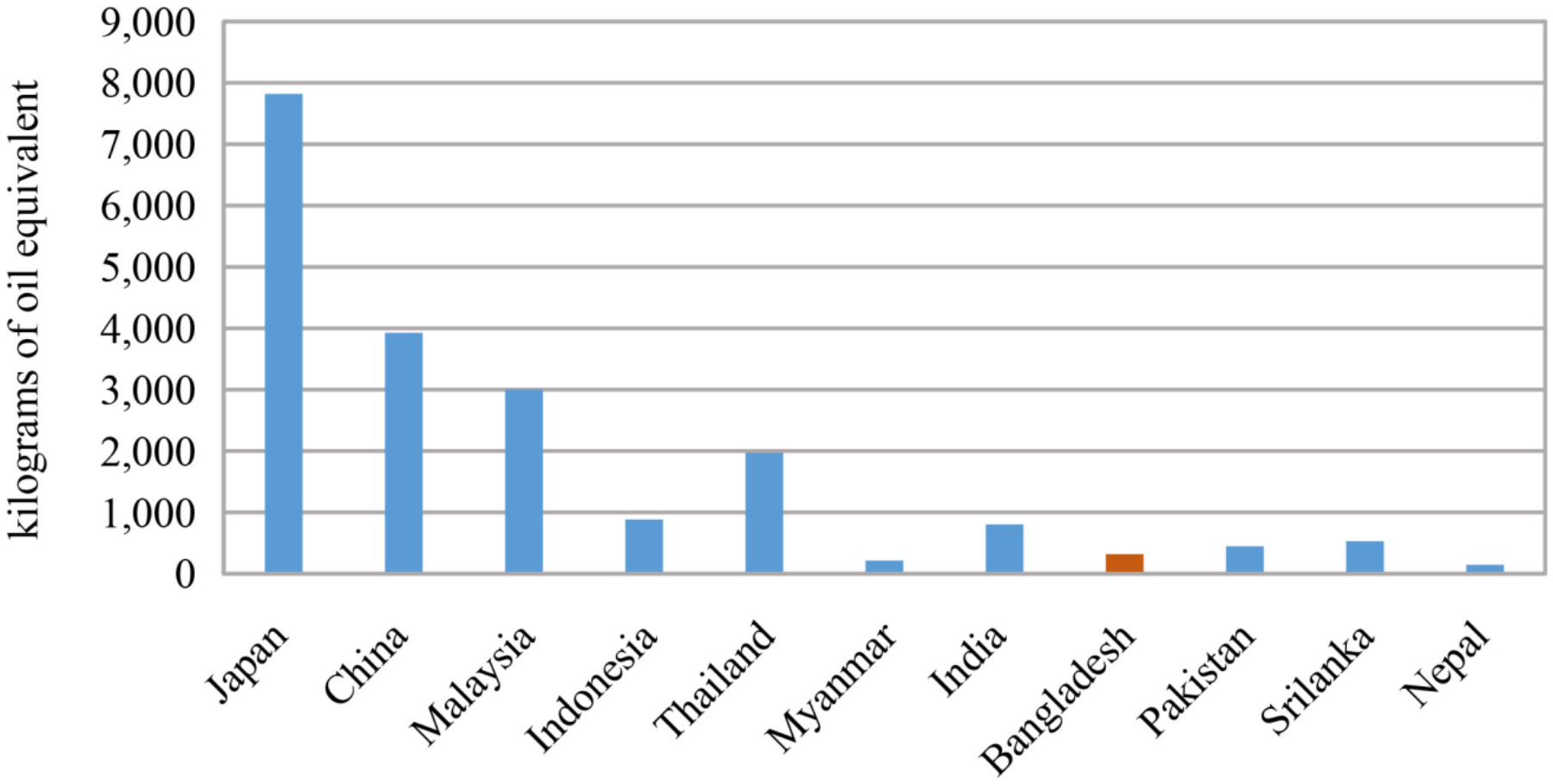
Source: TOP500 Supercomputer Database

Electronic structure software

Cite as: J. Chem. Phys. **153**, 070401 (2020); https://doi.org/10.1063/5.0023185
Submitted: 27 July 2020 . Accepted: 27 July 2020 . Published Online: 17 August 2020

Computational simulation has become accepted as a third mode of discovery, together with theory and experimentation,[1] and atomistic molecular simulation is one of the most widely used techniques in all of scientific computing. It has become standard in many disciplines, including physics, chemistry, biology, materials science, and mechanical engineering. Around 40% of supercomputing time is spent on molecular simulation (quantum chemistry and classical molecular dynamics).[2] Recognizing the growing importance of molecular simulation software, funding agencies across the globe have invested heavily in computational chemistry software development.

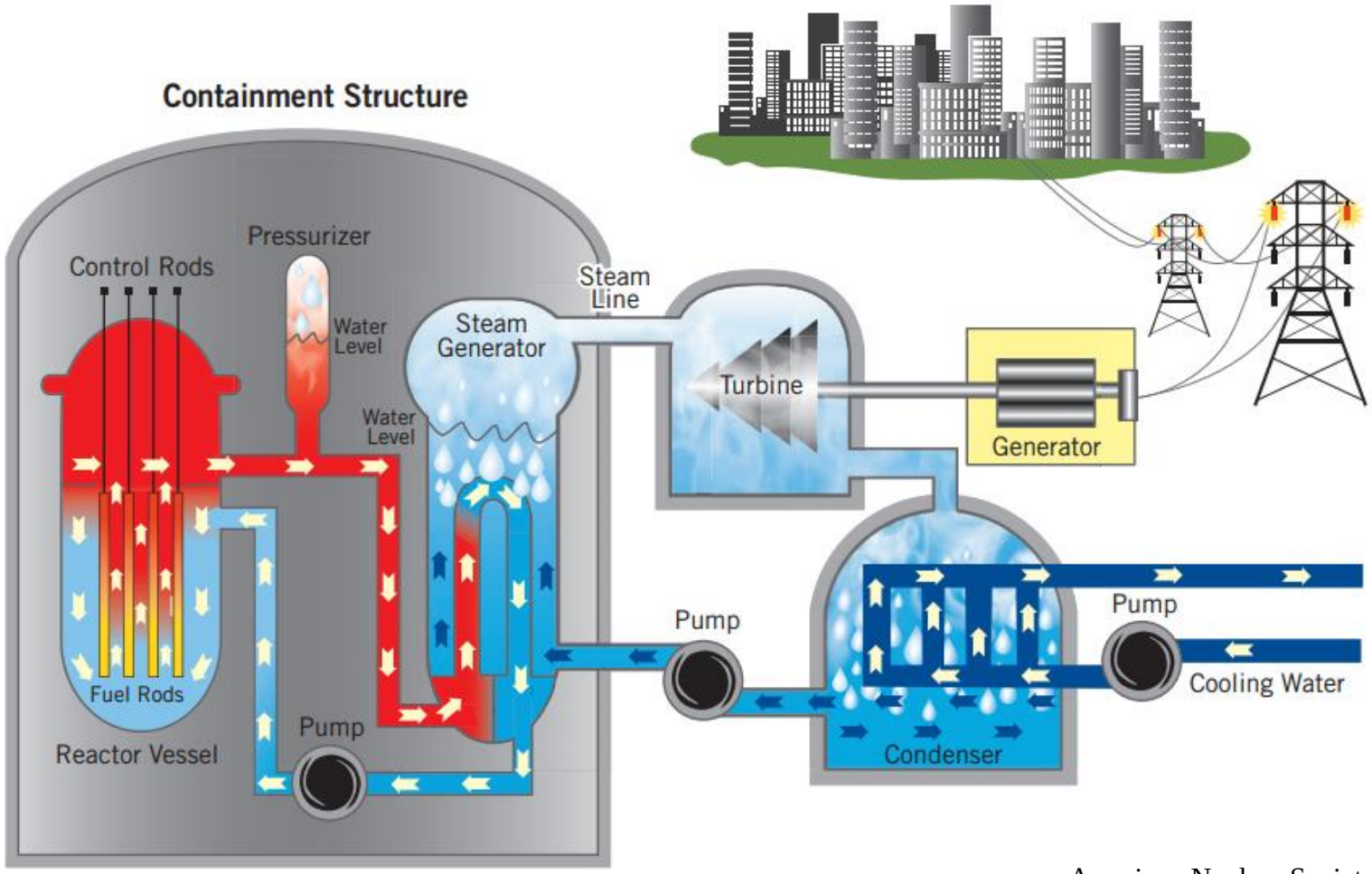
Energy consumption per capita



Energy consumption per capita in different countries of Asia.

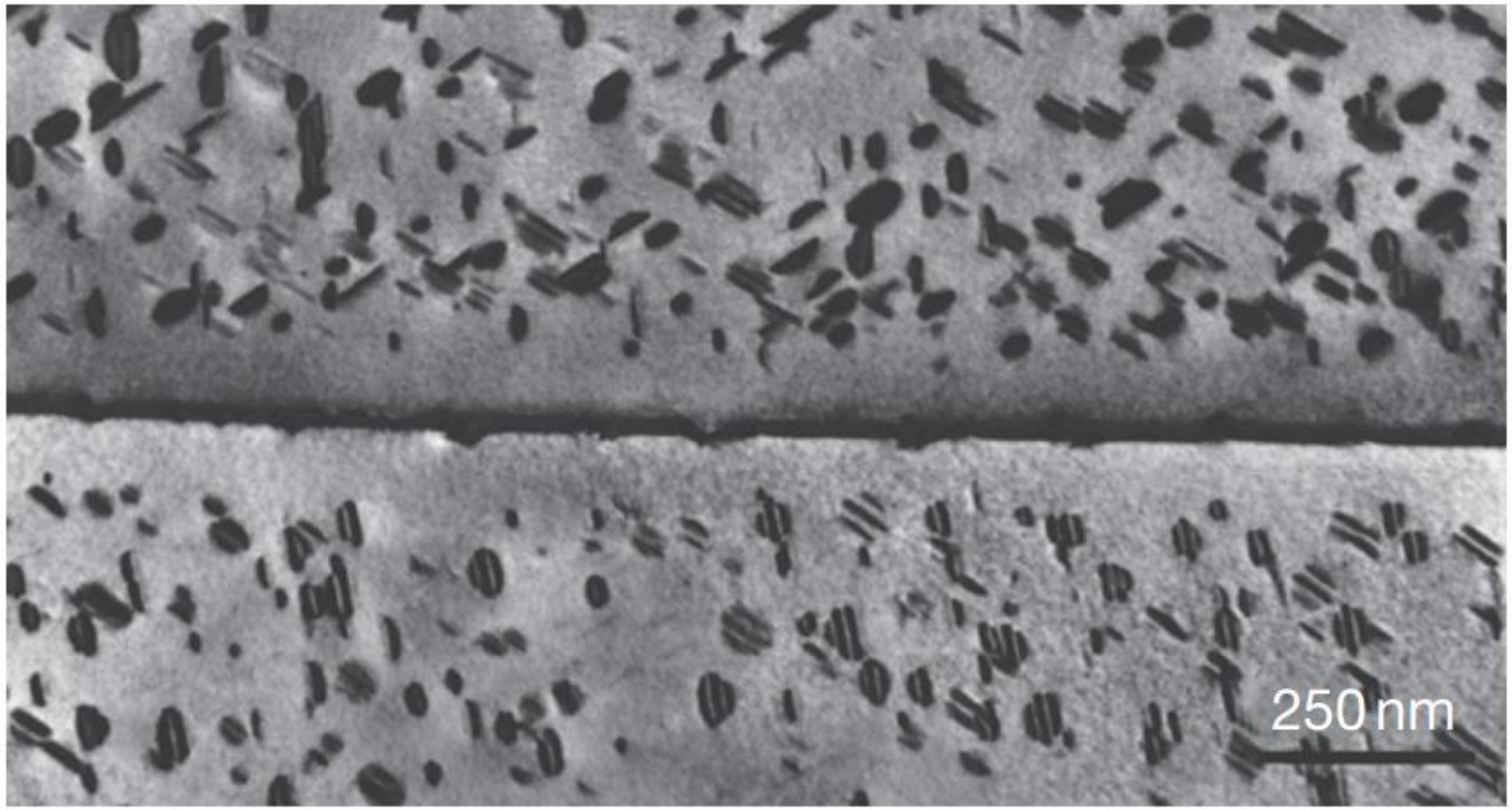
The World Bank Energy Use Report 2014

Nuclear technology & Bangladesh



American Nuclear Society

Radiation-induced precipitates



Rice et at., **Nucl. Mater.** 258–263, 1414–1419 (1998).

Goal of the project

- Learn and teach the use of modern technology
- Use ICT in research and education
- Develop new ICT based methodology for research
- Improve overall research quality of the department

Strategic Analysis

- DFT is the most accurate theoretical tool to estimate any physical, chemical and mechanical properties.
- Accuracy of DFT depends on the choice of exchange correlation function.
- Theoretical results need to be verified by experiments.

Publication in 2023

A. Allen, **Mohammad Abdur Rashid**, P. Rahe, S. P. Jarvis, J. N. O'Shea, J. L. Dunn & P. Moriarty, "Self-assembly and tiling of a prochiral hydrogen-bonded network: bi-isonicotinic acid on coinage metal surfaces", **Molecular Physics**, e2192824 (2023)

M. Naseri, D. R. Salahub, S. Amirian, H. Shahmohamadi, **Mohammad Abdur Rashid**, M. Faraji, N. Fatahi, "Multi-functional lead-free Ba_2XSbO_6 (X = Al, Ga) double perovskites with direct bandgaps for photocatalytic and thermoelectric applications: A first principles study", **Materials Today Communications** 35, 105617 (2023)

S. Jaman, M. B. Asfia, **Mohammad Abdur Rashid**, "Band gap engineering and enhanced optoelectronic performance by varying dopant concentration in $RbSr_{1-x}Sn_xCl_3$: Ab-inito study", **Physica B: Condensed Matter** [under review] (2023)

Publication in 2022

M. B. Asfia and **Mohammad Abdur Rashid**, "First principles calculations of structural, electronic and optical properties of Sn-doped ZnS", **Physica B: Condensed Matter** 646, 414335 (2022)

M. B. Asfia, S. Jaman and **Mohammad Abdur Rashid**, "Pressure induced band gap shifting from ultra-violet to visible region of $RbSrCl_3$ perovskite", **Materials Research Express** 9, 095902 (2022)

M. Naseri, D. R. Salahub, S. Amirian and **Mohammad Abdur Rashid**, "Computational investigation of Ba_2ZrTiO_6 double perovskite for optoelectronic and thermoelectric applications", **Journal of Solid State Chemistry** 314, 123385 (2022)

Mohammad Abdur Rashid, M. Saiduzzaman, A. Biswas and K. M. Hossain, "First-principles calculations to explore the metallic behavior of semiconducting lead-free halide perovskites $RbSnX_3$ (X = Cl, Br) under pressure", **European Physical Journal Plus** 137, 649 (2022)

M. B. Asfia and **Mohammad Abdur Rashid**, "First-Principles Study of Half Metallic Ferromagnetic and Optical Properties of Nb Doped Cubic ZnS using TB-mBJ Approximation", **Dhaka University Journal of Science** 69(3), 194-201 (2022)

Estimated Budget (BDT): **2,500,000.00**

No.	Item description	Quantity	Estimated unit price (BDT)	Total estimated cost (BDT)
1	High Performance Computer (HPC) with 64 threads and 128 GB RAM for DFT simulation	1	800,000.00	800,000.00
2	High Performance Computer (HPC) with 20 threads and 16 GB RAM for DFT simulation	5	250,000.00	1,250,000.00
3	Industrial grade online UPS (4 kVA) with 2 hours backup	1	300,000.00	300,000.00
4	DFT simulation software (WIEN2k)	1	70,000.00	70,000.00
5	Workshop	3	20,000.00	60,000.00
6	Stationary, Transport, etc			20,000.00
Total				**2,500,000.00**


Thank You