"My work involves the use of fundamental principles of physics through powerful computer simulations to determine how atoms and electrons are organized in space and time in a material. Using this information, we predict the behavior of the material, or properties of a material which are relevant to a wide range of applications from semiconductors in devices to the blades in jet engines."

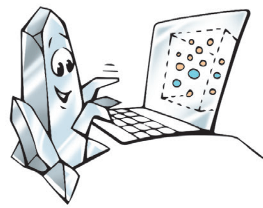
Umesh Waghmare

Professor, Theoretical Sciences Unit,
Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore

- B.Tech in Engineering Physics from Indian Institute of Technology, Bombay
- Ph.D. in Applied Physics from Yale University, New Haven
- Postdoctoral Research at Harvard University

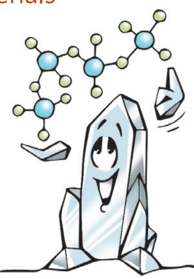
Prof. Umesh Waghmare is a rare theorist, who has demonstrated how state of the art first-principles calculations can be used on a wide range of materials to develop material-specific models through a systematic approach that starts at electronic scales, and used quantum or statistical mechanical analysis of these models to predict material behavior as a function of temperature and other external fields, while also assessing their potential for use in engineered devices.

Using computing wizardry to predict the behavior of materials

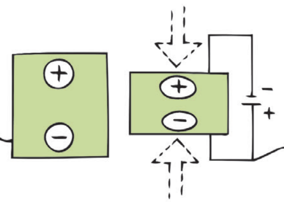


Prof. Umesh Waghmare works in the field of materials science. More specifically he works on the science of predicting how certain materials will work under specific conditions. Waghmare and his team do this using powerful computer simulation that use the fundamental principles of physics. This unique approach helps them determine the soundness of the theoretical approach while also verifying the experimentalists' approach.

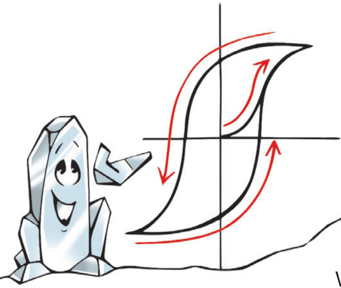
Human civilization has been divided into periods named for the materials most used by the people living during those times. Thus we have the Stone Age, the Iron Age and now we live in the semiconductor age. In each of these eras, man has tried to perfect the primary material used. Materials found in nature were taken, studied and improved upon in order to suit our purposes. This was how the area of materials science was born.



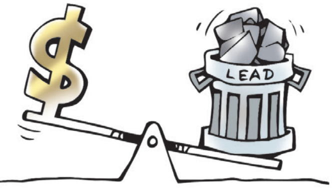
We now live in an age where materials are almost magical in their properties and advance technology in ways to which we are for the most part oblivious. Some of these materials, called smart materials, are ubiquitous. They can be found in everything from your devices to the blades in jet engines to the Mars rover to dental surgery and cardiac stents.



Smart materials possess a property called smart functionality. They can sense changes in their environment and respond accordingly. They have one or more properties that can be significantly changed in a controlled fashion by external stimuli such as stress, temperature, moisture, pH, electric or magnetic fields. Among the most used smart materials piezoelectrics, whose sub-class constitute ferroelectric materials.



Waghmare works with ferroelectrics. These materials have spontaneous electric dipoles which don't disappear even if you switch off the electric currents. But by applying electric field, the polarity can be reversed. In the digital age, ferroelectrics play a crucial role because they can be used to make non-volatile memory (memory is retained even if power is switched off). However, the problem with ferroelectrics is that they are costly and the technologically useful ones traditionally contain lead which is highly poisonous.



Waghmare and his team have been trying to find materials to replace the lead in ferroelectrics. Doing this experimentally would have meant huge costs. But with the modeling and computer simulation technique that Waghmare has conceived, they are able to predict the behaviors of the potential substitutes in a cost-effective manner. The challenge they face is that the new, improved material must have the same desirable properties as those of lead-containing compounds, such as 'phase transition and boundary', which means that by applying an electric field to the material you can get large flexibility in the response elicited from the material. Along a similar line, his group has predicted an atomically thin ferroelectric semiconductor and proposed dipolectronic device technology.