Preface

An International Workshop on Regularities, Classifications and Predictions of Advanced Materials was held at Centro di Cultura Scientifica A. Volta in Como, Italy, 13–15 April 1992. This specialized Workshop was attended by 44 participants from Europe, North America, Russian Federation and Japan.

The major topics discussed at this Workshop were:

- Quantum structure diagrams (QSD), structure maps and statistical maps; these diagrams are constructed by using several theoretically and empirically derived co-ordinates to systematize crystallographic data and chemical and physical properties of inorganic compounds.
- First principles calculations; the use of first-principles total energy electronic structure calculations to predict structural properties of materials.
- Structures and regularities; geometrical relationships, structural and property patterns and bonding factors.

The materials covered in this Workshop included an extensive range of conventional and advanced materials, including crystals, quasicrystals, clusters, layered structures (artificial and natural), alloys, ceramics, salts and intermetallics. Properties covered included ductility, machinability, weldability, ferroelectricity, superconductivity, magnetic and metal–insulator transitions.

This Workshop was a first in bringing together first-principles computational scientists, condensed matter physicists and database professionals. Connections between these areas can already be seen in the race to design new materials with specific properties. The applications of fundamental theoretical tools and empirical data bound together by computing technology will provide the necessary resources for developing new theories and providing a test bed for the modeling and simulation of new materials.

In summary, this Workshop highlighted the applications of QSDs and first-principles calculations in the field of material science. The papers in this issue are intended to communicate the excitement that pervades this dynamic area of condensed matter research. A new era of materials science has begun with materials systematics at its core. This Workshop seems to have captured the importance of this vital field and has already challenged the minds of many material scientists.

John R. Rodgers
Pierre Villars
Proceedings Editors

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