access the target functional inorganic porous crystalline materials can be described as:

1. A practical application, e.g., a specific catalytic reaction, raises detailed requirements for the structures with defined pore dimension, pore system, pore shape, active sites, etc.
2. The desired porous structures are then designed by computational methods.
3. By using computational modeling, the candidate SDA molecules are predicted for the given structures. Further data-mining techniques will predict the synthesis conditions for the target structures.
4. The synthesis is achieved by using various synthetic techniques under hydrothermal or solvothermal conditions. Especially, the combinatorial techniques will allow exploring in a large experimental space by means of the appropriate experimental design.
5. The structures of as-made materials are identified by comparing the experimental X-ray diffraction patterns with the simulated ones derived from the theoretical structures.
6. The application is eventually accessible by such a rational design and synthesis approach.

It is worth underscoring here that toward the rational synthesis of inorganic porous crystalline materials, there still remain a number of challenges ahead to achieve such a goal. Although great strides have been made in this area, future advances in understanding the formation mechanism at the molecular level are needed before the promise is fulfilled.

25.6 CONCLUDING REMARKS

The search for new inorganic materials has been moving from the empirical, trial-and-error methods of the past to a rational design philosophy. Our dream is to control chemically the self-assembly process of inorganic materials with predictable compositions, structures, and functionalities, and eventually to replace the classical trial-and-error strategy. This is, in fact, a long journey from possibility to reality. Despite the difficulties, this is the way where the synthetic chemists should concentrate. More research as well as untiring efforts should be driven along these directions.

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