

# Surrogate Modeling for Geometry Optimization in Material Design

## Problem

Find a stable configuration of atoms (geometry) for a molecule or solid: a geometry that minimizes the energy.

The optimization problem is:

$$\min_R E(R)$$

where

$E$  is the energy and

$R$  is the geometry (spatial coordinates of nuclei).

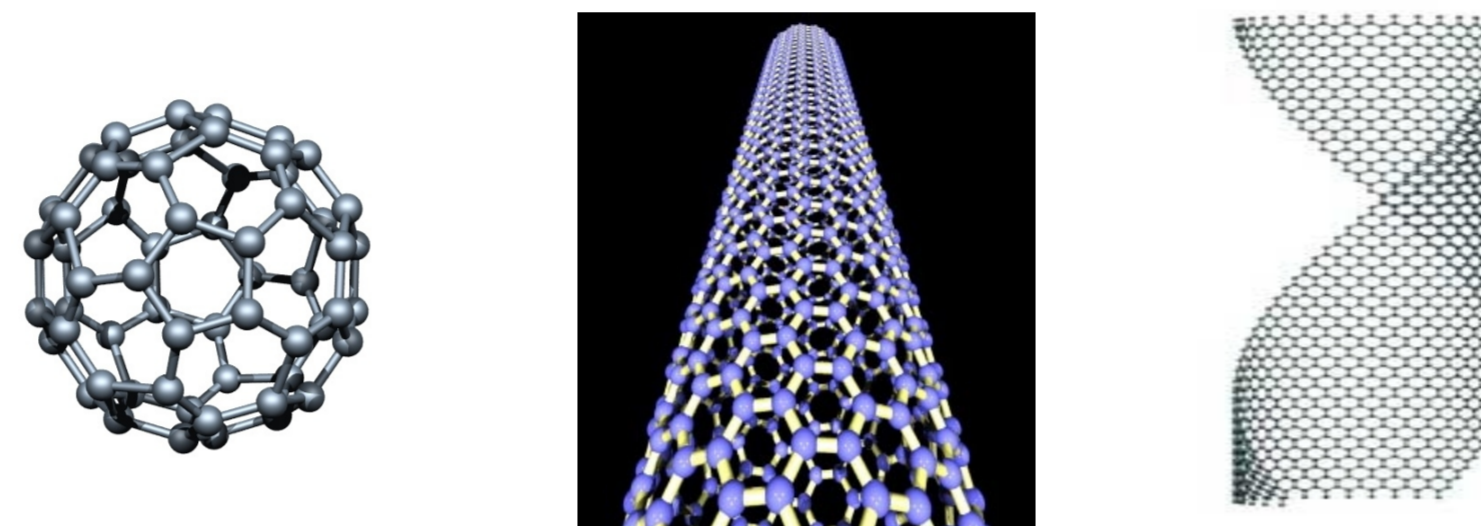
## Remarks

- Expensive objective function.
- Classic optimization methods require several evaluations of the energy and its gradient. Molecular-dynamics methods are expensive for large systems and are not robust for some materials.
- Existing approaches cannot use available data such as previously-computed energy values.

## Applications

Electronic structure calculations for the study and design of materials.

Example:  $C_{60}$  and nanotubes.



## Proposed Approach

Construct and minimize an inexpensive model (*surrogate*) of the objective function. In practice, one or two iterations of the following loop yield an acceptable solution.

**repeat**

Construct surrogate for  $E(R)$  using available energy values (design sites).

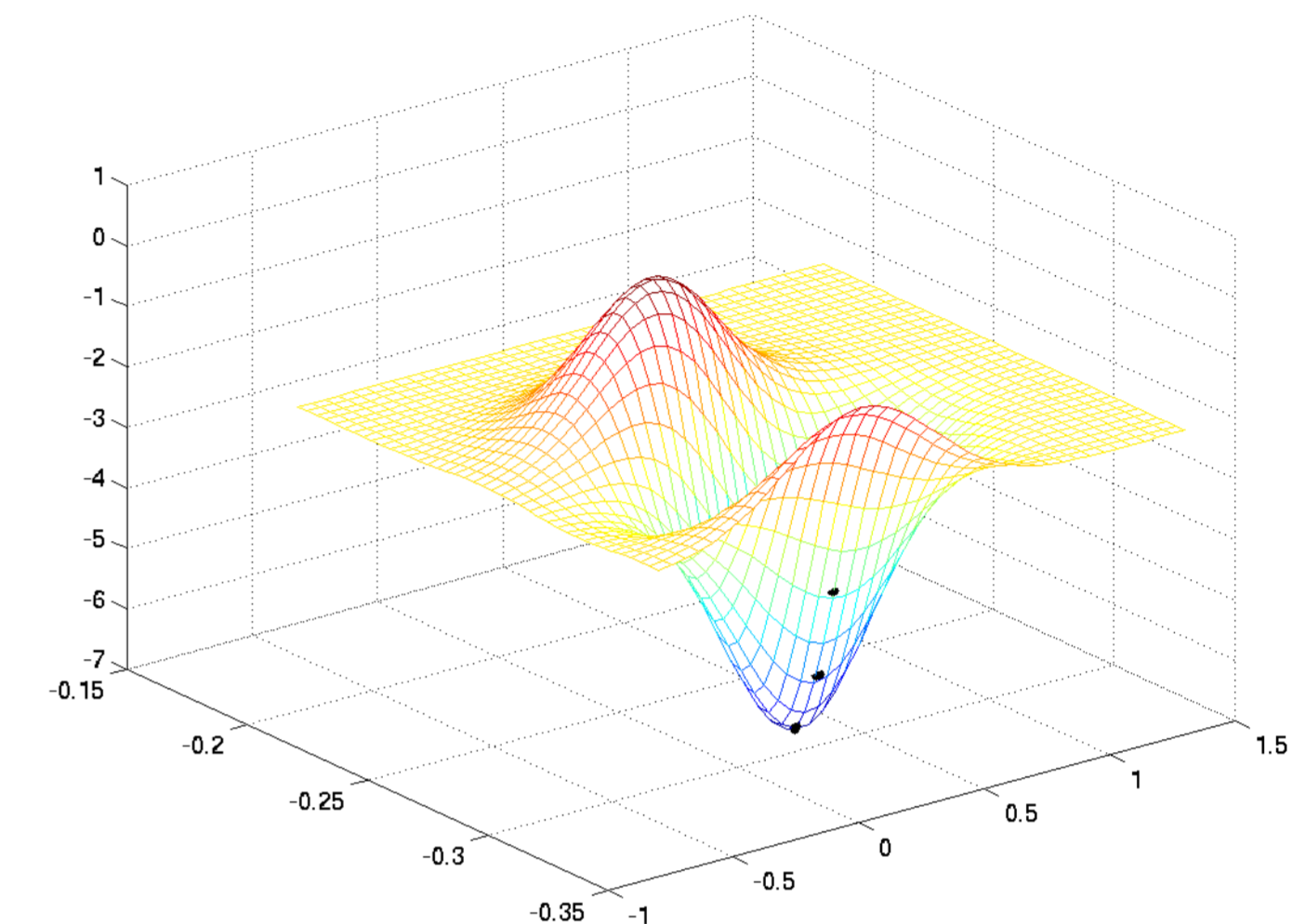
Compute minimizer  $R^*$  of surrogate.

Add  $\{R^*, E(R^*)\}$  to design sites.

**until** convergence

## Results

Energy surface for a 2D diamond sheet. The surrogate was computed with DACE [2].



## References

- [1] Y.B. Abraham. Optimization with surrogates for electronic-structure calculations, Master's Thesis, TR 2004-14, Department of Mathematics, Wake Forest University, Winston-Salem, North Carolina, USA, 2004.
- [2] S.N. Lophaven, H.B. Nielsen, and J. Sondergaard. DACE – A MATLAB Kriging Toolbox, version 2.0. IMM-TR-2002-12, Technical University of Denmark, Lyngby, August 2002.
- [3] M. Rojas, Y.B. Abraham, N.A.W. Holzwarth, and R.J. Plemmons. Surrogate Modeling for Geometry Optimization in Material Design. Proceedings of ICIAM 2007.

Images. SiH<sub>4</sub>: Chao Yang. C<sub>60</sub>, nanotubes: © www.ewels.info.



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