PCCP

Physical Chemistry Chemical Physics

$$E = f_1^2 \left(b_1^2 + \sum_{j=1}^{3} a_{j1}^{12} \cdot f_j^1 \left(b_j^1 + \sum_{i=1}^{2} G_i \cdot a_{ij}^{01} \right) \right)$$
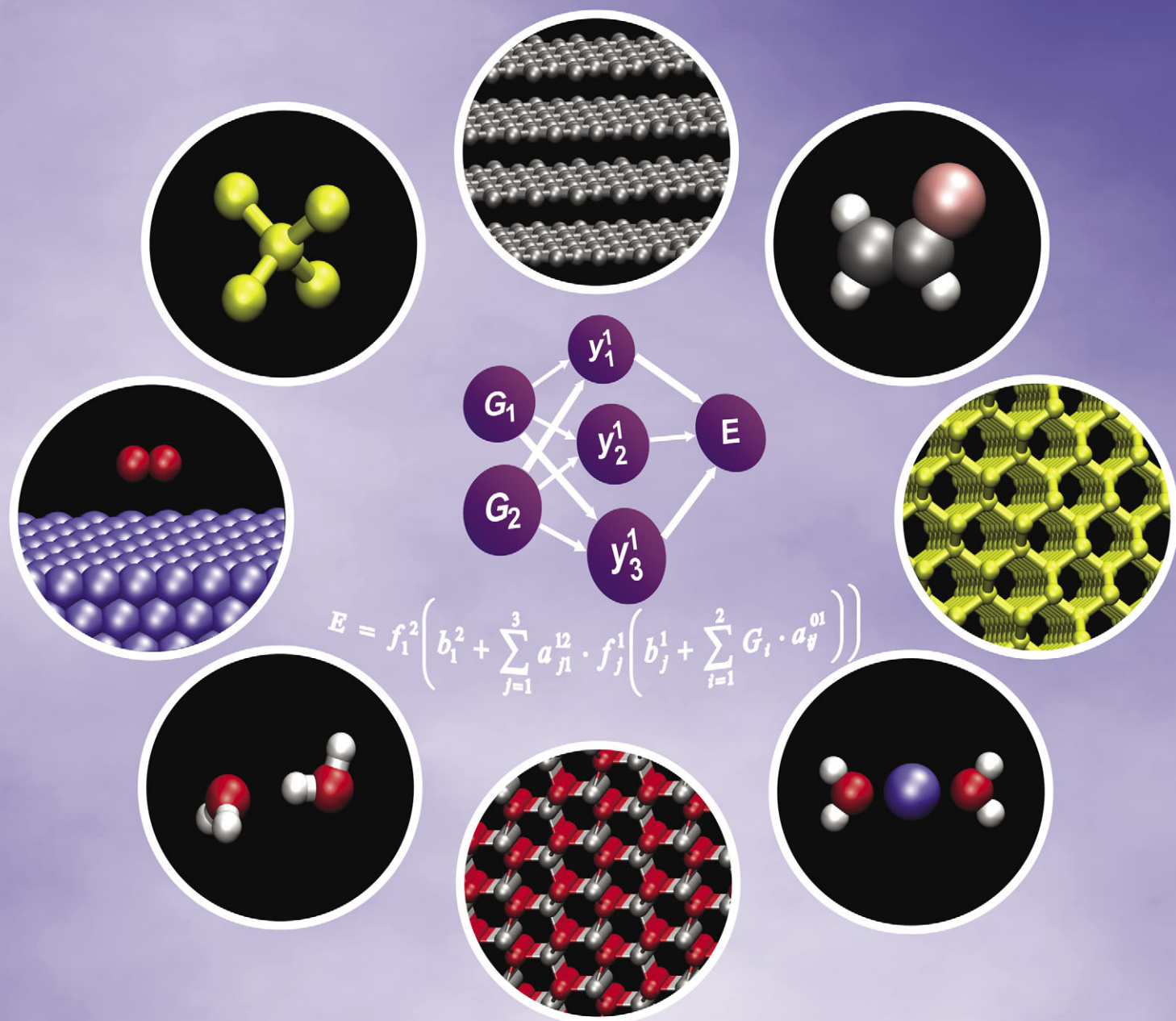
COVER ARTICLE
Behler
Neural network potential-energy
surfaces in chemistry: a tool for
large-scale simulations

COMMUNICATION
Bartlett *et al.*
The effect of Bi adsorption on CO
oxidation inside 1.8 nm Pt pores