

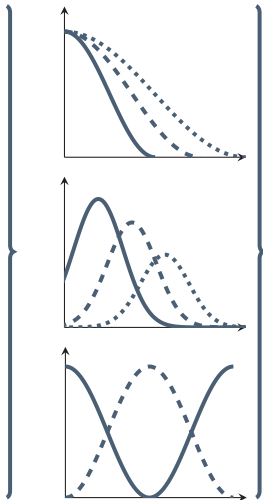
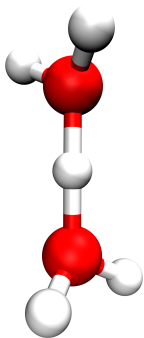
Structure \longrightarrow Energy

Symmetry
functions

Input
vectors

Atomic
NN

Atomic
energy



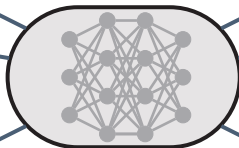
G_{H_1}

G_{H_2}

\vdots

G_{H_5}

NN_H



E_{H_1}

E_{H_2}

\vdots

E_{H_5}

NN_O



G_{O_1}

G_{O_2}

E_{O_1}

E_{O_2}

E_{tot}