メモ：(分子)グラフの機械学習

Machine Learning for Molecules and Materials NIPS 2017 Workshop の文献リスト

    http://www.quantum-machine.org/workshops/nips2017/

Neural Message Passing for Quantum Chemistry (ICML 2017) by google

    https://arxiv.org/abs/1704.01212

deepchemプロジェクト

    https://deepchem.io

SchNet

    https://github.com/atomistic-machine-learning/SchNet

Neural Graph Fingerprints (NIPS2015)

    https://github.com/HIPS/neural-fingerprint

Gated Graph Sequence Neural Networks (ICLR2016)

    https://github.com/yujiali/ggnn

Gated Graph Transformer Neural Network (ICLR2017)

    https://github.com/hexahedria/gated-graph-transformer-network

NMP実装(信頼性は要検証)

    https://github.com/priba/nmp_qc

Neural Graph FingerprintのKeras実装(信頼性は要検証)

    https://github.com/keiserlab/keras-neural-graph-fingerprint