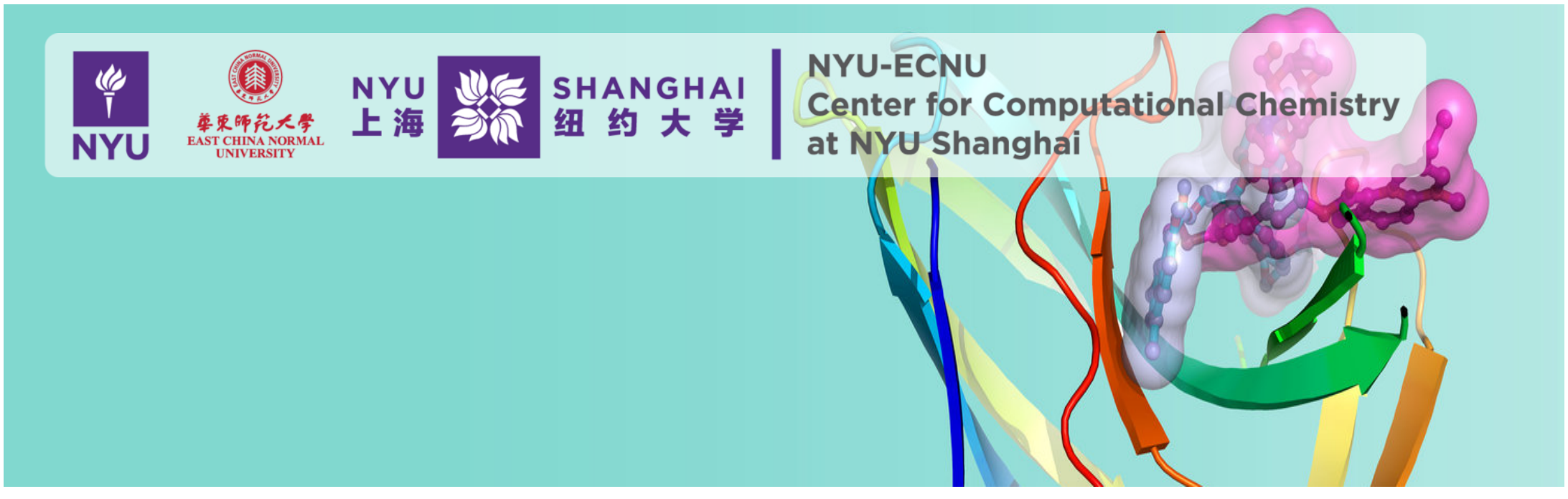

Course Schedule

Monday, June 12:

8:45 – 9:00: *Welcome and Introduction*
9:00 – 10:00: *Introduction to Machine Learning* (/s/lecture1.pdf) (Matthias Rupp)
10:00 – 10:20: *Coffee Break*
10:20 – 11:20: *Kernel-based Regression* (/s/lecture2.pdf) (Matthias Rupp)
11:20 – 12:30: *Dimensional Reduction, Feature Selection, and Clustering techniques* (/s/First_lesson_alex.pptx) (Alex Rodriguez)
12:30 – 14:00: *Lunch Break*
14:00 – 15:00: *Introduction to Neural Networks* (/s/Lecture_NN.pdf) (Mark Tuckerman)
15:00 – 15:30: *Coffee Break*
15:30 – 17:30: *Practical Session: Clustering with Feature Selection and Validation (Alex Rodriguez)*

Tuesday, June 13:

9:00 – 10:00: *Random Forests (/s/Lecture_RF_YingkaiZhang.pdf)* (Yingkai Zhang)
10:00 – 10:30: *Coffee break*
10:30 – 11:30: *Learning Curves, Representations, and Training Sets I* (/s/Lecture_LearningCurves_Anatole.pdf)(Anatole von Lilienfeld)
11:30 – 12:30: *Learning Curves, Representations, and Training Sets II* (/s/Lecture_LearningCurves_Anatole.pdf) (Anatole von Lilienfeld)
12:30 – 14:00: *Lunch Break*
14:00 – 15:00: *Review of Electronic Structure, Atomic, Molecular, and Crystal Representations* (/s/Lecture_ES.pdf) (Mark Tuckerman)
15:00 – 15:30: *Coffee Break*
15:30 – 17:30: *Practical Session: Learning Curves (Anatole von Lilienfeld)*

Wednesday, June 14:

9:00 – 10:00: *Predicting Properties of Molecules and Materials* (/s/lecture3.pdf) (Matthias Rupp)
10:00 – 10:30: *Coffee Break*
10:30 – 11:30: *Parameter Learning and Delta Learning (/s/Lecture_Parameters_Anatole.pdf)* (Anatole von Lilienfeld)
11:30 – 12:30: *Learning Electronic Densities* (Mark Tuckerman)
ML Models of Crystal Properties (Anatole von Lilienfeld)
12:30 – 14:00: *Lunch Break*
14:00 – 15:30: *Practical Session: Machine Learning and Property Prediction I (Matthias Rupp)*
15:30 – 16:00: *Coffee Break*
16:00 – 17:30: *Practical Session: Machine Learning and Property Prediction I (Matthias Rupp)*

Thursday, June 15:

9:00 – 10:00: *Machine Learning of Potential Energy Surfaces* (/s/Learning-Many-body-Potential-Energy-Functions-for-Condensed-Matter-Systems.pdf) (Ming Chen)
10:00 – 10:30: *Coffee Break*
10:30 – 11:30: *Machine Learning Based Enhanced Sampling* (/s/Learning-Collective-Variables-for-Enhanced-Sampling-Methods.pdf) (Ming Chen)
11:30 – 12:30: *Machine Learning of Free Energy Surfaces* (Mark Tuckerman)
12:30 – 14:00: *Lunch Break*
14:00 – 15:00: *Cluster-based Analysis of Molecular Simulations* (/s/Second_lesson_alex.pptx) (Alex Rodriguez)
15:00 – 15:30: *Coffee Break*
15:30 – 17:30: *Practical Session: Neural Network Learning of Free Energy Surfaces (Mark Tuckerman)*

Friday, June 16:

9:00 – 10:00: *Development of Protein-ligand Scoring Functions* (/s/Lecture_Docking_YingkaiZhang.pdf) (Yingkai Zhang)
10:00 – 10:30: *Coffee Break*
10:30 – 11:30: *Machine Learning in Structural Biology (/s/Machine_learning_in_StrBio_share-l4ge.pdf) I* (Yang Zhang)
11:30 – 12:30: *Machine Learning in Structural Biology II* (Yang Zhang)
12:30 – 14:00: *Lunch Break*
14:00 – 15:30: *Practical Session: Random Forests and Scoring Functions (Yingkai Zhang)*
15:30 – 16:00: *Coffee Break*
16:00 – 17:30: *Practical Session: Machine Learning for Structural Bioinformatics (Yang Zhang)*

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