

Predicting Real, Optimized Materials (PROM)
 Program Kickoff Meeting at Caltech
 California Institute of Technology, 115 Beckman Institute (building 74)
 July 18-19

18-Jul		Overview and Planning
8:00 AM	8:15 AM	0:15 Coffee
8:15 AM	8:45 AM	0:30 Welcome, vision Carey Schwartz
8:45 AM	9:05 AM	0:20 Caltech Overview Goddard
9:05 AM	9:35 AM	0:30 Reactive FF van Duin
9:35 AM	10:05 AM	0:30 FE/TE Cagin
10:05 AM	10:20 AM	0:15 Coffee break
10:20 AM	10:40 AM	0:20 NLO-TD-DFT Tahir-Kheli
10:40 AM	11:10 AM	0:30 TE/NLO von Allmen
11:10 AM	11:40 AM	0:30 ISP estimation/FE Strachan
11:40 AM	12:00 PM	0:20 mesoscale ferro Cuitino
12:00 PM	12:45 PM	0:45 Lunch
12:45 PM	1:05 PM	0:20 Software Integration Meulbroek
1:05 PM	1:35 PM	0:30 Top-down integration Klimeck
1:35 PM	1:55 PM	0:20 Applications to HE Vashishta
1:55 PM	2:15 PM	0:20 Visualization Nakano
2:15 PM	2:35 PM	0:20 Scaling Methods Kalia
2:35 PM	3:20 PM	0:45 LANL Effort Galli
3:20 PM	3:35 PM	0:15 coffee
3:35 PM	3:50 PM	0:15 NLO Marzari
3:50 PM	4:20 PM	0:30 inverse molecular des Beratan
4:20 PM	4:30 PM	0:10 Spintronics / TE Zunger (WAG)
4:30 PM	4:40 PM	0:10 Higher-dimension scal Beylkan (WAG)
4:40 PM	4:50 PM	0:10 equation-free comple Kevrekidis (WAG)
4:50 PM	5:20 PM	0:30 Wrap-up/Discussion Schwartz
19-Jul		Workshops and Planning
9:00 AM	10:00 AM	1:00 general discussion, assignments to subgroups
10:00 AM	12:00 PM	2:00 subgroups meet and discuss
12:00 PM	1:00 PM	1:00 lunch
1:00 PM	3:30 PM	2:30 continued discussions in subgroups
3:30 PM	4:00 PM	0:30 Final Summary