

**ACADEMIC AFFAIRS OFFICE
INDIAN INSTITUTE OF TECHNOLOGY ROORKEE**

No. Acd./ 3160 /IAPC-78

Dated: February 05 , 2020

Head, Department of Metallurgical & Materials Engineering
(through e-mail)

The IAPC in its 78th meeting held on 31.12.2019 vide **Item No. 78.2.2 (1)** considered the proposal to revise curriculum of PCC MTN-502: Modelling, Simulation and Computer Applications.

The IAPC accepted the proposal with minor modifications. The modified syllabus is attached as **Appendix-A**.


Assistant Registrar (Curriculum)

Encl: as above

Copy to (through e mail):-

1. All faculty
2. All Heads of Departments/ Centres
3. Dean, Academic Affairs
4. Associate Dean of Academic Affairs (Curriculum)
5. Channel I/ Academic webpage of iitr.ac.in

List of Practicals:

1. Defect energy calculation using Molecular Statics
2. Molecular Dynamics simulation of melting
3. Simulations of deformation using Molecular Dynamics
4. Metropolis Monte-Carlo study of the Ising model
5. Employing Q-state Potts model to simulate grain growth
6. Phase-field simulation of spinodal decomposition

11. Suggested Books:

S.No.	Name of Author (s) / Book/ Publisher	Year of Publication
1.	Lesar R., An introduction to computational material science – Fundamentals to Applications, Cambridge University Press	2013
2.	Landau D. P., and Binder K., A Guide to Monte-Carlo Simulation in Statistical Physics, Cambridge University Press	2014
3.	Frenkel D., and Smit B., Understanding Molecular Simulation, Academic Press	2001
4.	Provatas N., and Elder K., Phase-field methods in Material Science and Engineering, Wiley-VCH	2011