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F. No. 1546-21/IITRPR/GTE/PS/

PROCUREMENT PLAN FOR THE NEXT 5 YEAR

S. No.	Name of the Equipment	Faculty Name	Use of the Equipment/Software	Estimated Quantity
01	Vienna Ab initio Simulation Package (VASP)_Density Functional Theory (DFT) Software (Already sent for approval)	Dr Neha Sardana, DMME	Simulations	1 set of license
02	VASP Software GmbH (Already sent for approval)	Dr Arghya Banerjee, Chemical Engineering	The above software is going to be used for performing first principles DFT calculations. These calculations has multiple applications in the fields of materials science, catalysis, chemical engineering etc.	Permanent license for 6 users (in a single group)
03	Laser Diode Setup With Drivers (Already sent for approval)	Dr Neha Sardana, DMME	Experimental light source	1 set
04	VASP Software GmbH (To be procured in future)	Dr. Tarak Mondal, Chemical Engineering	The VASP software will be used to gain an in-depth knowledge of the process chemistry so as to identify the best suited catalyst, identification of possible reaction mechanism, products and by-products for our different research work using DFT study.	1 licence
05	VASP Software GmbH (To be procured in future)	Dr Sarang Gumfekar, Chemical Engineering Department	Screening of porous materials for interactions with water contaminants and gas separation analysis. General applications- water treatment, materials screening, gas separation	1